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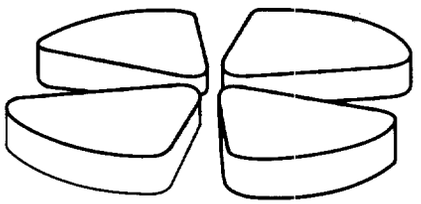

Solving the Generalized Langevin Equation with the Algebraically Correlated Noise

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Abstract

We solve the Langevin equation with the memory kernel. The stochastic force possesses algebraic correlations, proportional to $1/t$. The velocity autocorrelation function and related quantities characterizing transport properties, are calculated at the assumption that the system is in the thermal equilibrium. Stochastic trajectories are simulated numerically, using the kangaroo process as a noise generator. Results of this simulation resemble Lévy walks with divergent moments of the velocity distribution. We consider motion of a Brownian particle, both without any external potential and in the harmonic oscillator field, in particular the escape from a potential well. The results are compared with memory-free calculations for the Brownian particle.

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I. INTRODUCTION

Stochastic equations are often regarded as an effective description of a complicated high-dimensional system. Fast varying variables are substituted by a fluctuating force and the stochastic equation possesses only few degrees of freedom. However, such a procedure destroys in general the Markovian property of the original system [1]. Consequently, the stochastic force put into the effective equation must have a finite correlation time. The non-Markovian behaviour is especially prominent in nonlinear dynamical systems possessing a complex structure of the phase space, where chaotic regions coexist with regular, stable structures. Trajectories stick to islands of stability and only slowly penetrate cantori. They consist then of long segments corresponding to free paths, interrupted by intervals of frequent and rapid changes of direction. This kind of motion is known as Lévy flights (walks). Processes exhibiting Lévy flights are scale-invariant and have fractal properties: they are usually characterized by divergent moments [2]. Specific transport properties like the anomalously enhanced diffusion can be accounted for the existence of long jumps. The velocity autocorrelation function (VAF), $C(t) = \langle \mathbf{v}(0)\mathbf{v}(t) \rangle$, depends algebraically on time and the mean squared displacement rises faster then lineary with time [3]. Those quantities are strictly connected to the statistics of free paths [4].

Slowly decaying correlations are known in various phenomena including the chemical reactions in solutions [5] , ligands migration in biomolecules [6] , atomic diffusion through a periodic lattice [7] , Stark broadening [8] and many others. The power-low autocorrelation functions have been also found in the molecular dynamics [9] devised to describe nuclear collisions. From the point of view of transport phenomena, models of this kind can be traced back to a very simple system: the Lorentz gas of periodically distributed scatterers. A particle can move freely in such a lattice for very long time intervals giving rise to long tails of VAF, proportional to $1/t$. The autocorrelation of force in the molecular dynamics has the same form. The mean squared displacement $\langle \mathbf{r}^2 \rangle$ is proportional to $t \ln t$, then the diffusion coefficient diverges logarithmically. If one passes on to quantum mechanics and

takes into account the antisymmetrization effects [10], all above observations still hold.

To study transport phenomena of a system with known fluctuation properties, it is appropriate to apply the Langevin formalism, avoiding intricacies of many-body dynamics. Recently, we have addressed the Langevin problem for algebraic correlations [11] solving the two-dimensional stochastic equation:

$$\begin{aligned} \frac{d\mathbf{r}}{dt} &= \mathbf{v} \\ m\frac{d\mathbf{v}(t)}{dt} &= -\beta\mathbf{v}(t) - \frac{\partial V(\mathbf{r})}{\partial \mathbf{r}} + \mathbf{F}(t) \quad , \end{aligned} \tag{1}$$

where the potential V generates a conservative force, β is the friction constant, and the external noise (stochastic force) $\mathbf{F}(t)$ has algebraically decaying correlations:

$$\begin{aligned} \langle \mathbf{F}(0)\mathbf{F}(t)\rangle &\sim 1/t \\ \langle \mathbf{F}(t)\rangle &= 0 \ . \end{aligned} \tag{2}$$

The stochastic force $\mathbf{F}(t)$ has been assumed as a time series generated by a deterministic, but chaotic, dynamical system, namely as proportional to the velocity of particle in the two-dimensional periodic Lorentz gas (the generalized Sinai billiard). In that approach, the friction force is an intrinsic property of the system, unrelated to the properties of the driving noise. Hence, the fluctuation - dissipation theorem is not fulfilled. Nevertheless, for any initial condition in the Langevin equations, the system drives towards an asymptotic stable state with the constant $\langle \mathbf{v}^2 \rangle$. It has been found that in the absence of external potential, the mean squared displacement $\langle \mathbf{r}^2 \rangle(t)$ grows as $t \log t$, thus the diffusion coefficient is infinite. A study of the particle escape from a parabolic potential well has revealed important differences, compared to the case of fast decaying correlations. The energy distributions have a pronounced peak corresponding to the particles which are associated with long trajectories in the adjoined billiard and leave the potential well without any change of chaotic force value. This peak is superimposed on the Gaussian distribution. The Gaussian shape of the energy distribution, in contrast to the Maxwellian exponential shape, is connected with particles dwelling inside the potential well for a long time, never reaching the equilibrium state.

In turn, the probability that the particle remains inside the well (the survival probability) depends on time as $1/t$, in the large t limit.

The above approach is an approximation because it neglects memory effects. In fact, a properly formulated Langevin problem emerging as a coarse graining over a set of hidden variables must contain a velocity dependent friction term [12]. For that purpose, Kubo [13] postulated instead of (1), a phenomenological integro-differential equation:

$$m\frac{d\mathbf{v}(t)}{dt} = -m\int_0^t K(t-\tau)\mathbf{v}(\tau)d\tau - \frac{\partial V(\mathbf{r})}{\partial \mathbf{r}} + \mathbf{F}(t) \tag{3}$$

where $K(t)$ represents the retarded friction kernel. This equation implies the dissipation-fluctuation theorem, linking properties of the stochastic force (amplitude, correlation time) and characteristics of a heat bath with which the system remains in the equilibrium.

Memory effects have important physical consequences. The meaning and significance of history-dependent frictional resistance for fluid dynamics has been realized already at the beginning of the century by Boussinesq [14]. In the framework of the reaction-rate theory [15], memory effects modify substantially the Kramers result [16] for the escape rate from metastable states. In turn, the kinetic equation which is non-Markovian does not conserve energy due to memory effects (the collision broadening) [17]. As a result, the influence of collisions on the time evolution of the distribution function is diminished [18] and the initial distribution survives longer. The similar change of the relaxation time has been obtained from the quantum kinetic equation [19]. One can then expect important consequences on problems formulated in terms of the Boltzmann-Langevin equation [20] . In nuclear dynamics, taking into account memory effects is crucial because systems considered are small [21].

The molecular dynamics can serve as a simple model of fluid, the molecules being represented as hard spheres. Then one can also expect algebraic correlations, similarly as for the Lorentz gas. Indeed, Alder and Wainwright [22] have shown by a direct numerical integration of the Navier-Stokes equation, that the diffusion coefficient diverges and the VAF has the algebraic tail. In the two-dimensional case it approaches t^{-1} , whereas in three dimen-

sions: $t^{-3/2}$. Solving the Langevin equation with the retarded frictional resistance, derived by Boussinesq [14]), Mazo [23] has found that the autocorrelation function of the random force is proportional to $t^{-3/2}$ for large t. Exponents determining autocorrelation functions in hydrodynamics depend mainly on the dimensionality of the system and are insensitive to both the interaction and the shape or size of the Brownian particle. Recently, the long-time Brownian motion has been studied in the framework of the linearized hydrodynamics [24]. It has been found that in two dimensions the VAF approaches asymptotically $1/t$ for translational Brownian motion and $1/t^2$ for rotational one.

In this paper we present solutions of Eq.(3) for the noise with the algebraic autocorrelation function. Some averaged quantities, like the VAF, can be easily derived from (3) without defining details of the stochastic force, providing the stochastic system is in the thermal equilibrium. We do that in Sec.II, starting from usual assumptions, originally stated by Kubo [13]. The main purpose of this work is, however, to solve the GLE directly by simulating trajectories numerically. A possibility of such simulation is important for modeling physical processes. In Sec.III we present a method of generation of the stochastic force with given, e.g. algebraic, correlations. For this purpose we utilize a specific generalization of the random walk, a Markov process known as the kangaroo process. Inserting a time series generated in that way into (3) and solving the equation, we get a trajectory. Averaging over statistical ensemble allows to determine statistical properties of the system (Sec.IV). In Sec.V we consider the Brownian motion in the harmonic oscillator field and in Sec.VI we summarize the most important results of this work.

II. THE VELOCITY AUTOCORRELATION FUNCTION FOR THE EQUILIBRIUM STATE

We start with the equation (3) providing $V(\mathbf{r}) = 0$. Let the stochastic force $\mathbf{F}(t)$ satisfy the conditions:

$$\langle \mathbf{F}(t) \rangle = 0 \tag{4}$$

and

$$\langle \mathbf{v}(0)\mathbf{F}(t) \rangle = 0. \tag{5}$$

The condition (5) can be interpreted as a manifestation of the causality [25]. We assume that the system is in the equilibrium with the heat bath of temperature T. Multiplying the Eq.(3) by $\mathbf{v}(0)$ and averaging over the equilibrium ensemble we get :

$$m\frac{d}{dt}\langle \mathbf{v}(0)\mathbf{v}(t) \rangle = -m\int_0^t K(t-\tau)\langle \mathbf{v}(0)\mathbf{v}(\tau) \rangle d\tau + \langle \mathbf{v}(0)\mathbf{F}(t) \rangle. \tag{6}$$

From (5), the last term vanishes. The above equation can be solved to obtain the VAF. Using Laplace transforms, one gets [26]:

$$\widetilde{C}(s) = \frac{\langle \mathbf{v}^2 \rangle}{s + \widetilde{K}(s)} \tag{7}$$

where tilde denotes, from now on, the Laplace transform: $\widetilde{f}(s) \equiv \mathcal{L}[f(t)]$. Similarly, multiplying the generalized Langevin equation by $\mathbf{F}(0)$ and using (7) one obtains [26] the fluctuation-dissipation theorem:

$$\widetilde{K}(s) = \langle \mathbf{F}(0)\mathbf{F}(s) \rangle / (m^2 \langle \mathbf{v}^2(0) \rangle) \tag{8}$$

where $\langle \mathbf{F}(0)\mathbf{F}(s) \rangle = \mathcal{L}[\langle \mathbf{F}(0)\mathbf{F}(t) \rangle]$. Since the system is supposed to be in the equilibrium state, characterized by the temperature T, hence $\langle \mathbf{v}^2(0) \rangle = T/m$. Then inverting (8) allows to express the friction kernel by the noise autocorrelation function $C_F(t) = \langle \mathbf{F}(0)\mathbf{F}(t) \rangle$:

$$K(t) = \langle \mathbf{F}(0)\mathbf{F}(t) \rangle / mT. \tag{9}$$

The generalized Langevin equation with the stochastic force correlated algebraically has been extensively studied in connection with the motion of Brownian particles in a viscous fluid. Chow and Hermans [27] have solved Eq.(6) for noise correlations, i.e. memory kernels, proportional to $t^{-3/2}$, $t > 0$. They found $C(t) \sim t^{-3/2}$ asymptotically, for large times.

Let us consider the following noise autocorrelation function:

$$C_F = \begin{cases} \alpha/\epsilon & t \leq \epsilon \\ \alpha/t & t > \epsilon \end{cases} \tag{10}$$

where ϵ is a small number. Without the loss of generality, the constant α will be assumed equal one in the numerical calculations.

Using (9), we calculate the Laplace transform of the kernel. Formula (7) takes the form:

$$\tilde{C}(s) = \frac{T/m}{s + \alpha\,(1 - \mathrm{E}i(-\epsilon s))/mT} \tag{11}$$

where $\mathrm{Ei}(z)$ denotes the integral exponential function defined by:

$$\mathrm{E}i(z) = \int_{-\infty}^{z} \mathrm{e}^{x}/x \; dx \tag{12}$$

and the integral is calculated on an arbitrary path on the plane x, cut along the positive real half-axis. To determine the VAF, we have to invert the Laplace transform, performing the integral:

$$C(t) = \mathcal{L}^{-1}[\tilde{C}(s)] = \frac{1}{2\pi i} \int_{-i\infty+\sigma}^{+i\infty+\sigma} \tilde{C}(z)\,\mathrm{e}^{tz} \; dz \quad . \tag{13}$$

Details of the derivation are explained in the Appendix. The final result reads:

$$C(t) = \frac{T}{m}\,\chi(t) \qquad (t > 0) \tag{14}$$

where

$$\chi(t) = \mathrm{e}^{-at}\,(c_1 \sin bt + c_2 \cos bt) - \tag{15}$$

$$-mT/\alpha \int_0^{\infty} \frac{\mathrm{e}^{-tx}\; dx}{(mTx/\alpha + \mathrm{E}i_1(\epsilon x) - 1)^2 + \pi^2} \quad .$$

In the above expression the constants a, b, c_1 and c_2 depend both on ϵ and T. The modified integral exponential function $\mathrm{Ei}_1(x)$ is defined by the following expansion:

$$\mathrm{E}i_1(x) = \gamma + \ln x + \sum_{n=1}^{\infty} x^n/n!\,n, \quad x > 0 \tag{16}$$

where $\gamma = 0.5772157\ldots$ is the Euler constant.

The Laplace transform in the expression (15) can be easily evaluated numerically. Fig. 1 shows $C(t)$ for temperatures $T = 1, 2$ and $\epsilon = 5 \cdot 10^{-3}, 10^{-2}$. For all presented cases, the curves initially fall rapidly to negative values and then approach zero from below. For large t, the tail is algebraic with numerically estimated exponent equal -1.18. This kind of asymptotic behaviour is called "the Lorentz tail" and is typical in the molecular dynamics [28]. It can be observed at all densities of random scatterers and for all sorts of their types and arrangements. For example, the same shape of VAF has been found by Rahman [29] in molecular-dynamical simulation of interacting particles motion in the liquid argon.

This shape of the VAF cannot be achieved for the fast decaying noise correlations. For comparison, let us consider $C_F(t) = \alpha \exp(-2\bar{\gamma}t)$. Then (7) becomes:
$\tilde{C}(s) = T/m\ (s + 2\bar{\gamma})/(s(s + 2\bar{\gamma}) + \alpha/mT)$. Inverting this Laplace transform, we get for the VAF the following expression:

$$C(t) = T/m\ \times \begin{cases} 1/2\sqrt{-\Delta}\ \left(B\mathrm{e}^{-At} - A\mathrm{e}^{-Bt}\right) & \Delta < 0 \\ \mathrm{e}^{-\bar{\gamma}t}\,(\bar{\gamma}\,t + 1) & \Delta = 0 \\ \mathrm{e}^{-\bar{\gamma}t}/\sqrt{\Delta}\ \left(\bar{\gamma}\,\sin\sqrt{\Delta}\,t + \sqrt{\Delta}\cos\sqrt{\Delta}\,t\right) & \Delta > 0 \end{cases}$$

where $A = \bar{\gamma} - \sqrt{-\Delta}$, $B = \bar{\gamma} + \sqrt{-\Delta}$ and $\Delta = \alpha/(mT) - \bar{\gamma}^2$. Thus the exponential tail of the VAF found in this case is quite different from the tail found for the algebraic noise correlations. For small $\bar{\gamma}$, the tail may become negative but then it oscillates around zero with the exponentially diminishing amplitude.

Knowing the VAF, one can calculate the mean square displacement applying the identity:

$$\langle \mathbf{r}^2 \rangle(t) = 2 \int_0^t (t - \tau) C(\tau) d\tau\ . \tag{17}$$

Hence, the diffusion coefficient:

$$\mathcal{D} = \frac{1}{2} \lim_{t->\infty} \frac{d}{dt} \langle \mathbf{r}^2 \rangle(t)$$

is given by

$$\mathcal{D} = \int_0^\infty C(t)dt \,. \tag{18}$$

The diffusion coefficient assumes a finite value for the algebraic correlations. This can be checked by inserting (14) and (15) into (18), changing the order of integration and expanding the Ei_1 function. Thus with the assumptions made in this Section, the GLE does not imply any kind of the anomalous diffusion for the noise correlated as $1/t$. However, it is not obvious that the GLE with algebraic correlations gives the velocity distribution with the convergent second moment, i.e. the system is always able to reach the thermal equilibrium. We will address this general problem in a separate paper. In the following, we solve directly the GLE with a concrete, specifically prescribed stochastic force and show that in that case the velocity variance can diverge.

III. GENERATION OF THE STOCHASTIC FORCE

For that purpose we apply a stochastic process called "the kangaroo process" (KP). It is defined [30] as a stepwise random function $m(t)$: $m(t) = m_i$ in the time interval $t_i \leq t < t_{i+1}$. The length of intervals of constant m, i.e. the frequency of jumping times $\nu(m)$, is a function of the value of the process itself. The KP is a stationary Markov process. The probability that the KP at time Δt is between m and $m + dm$, knowing that it was equal m' at time $t = 0$, is given for infinitesimal time intervals Δt by :

$$P_{KP}(m, \Delta t \mid m', 0) = \{1 \; - \; \nu(m')\Delta t\} \; \delta(m - m') + Q(m)\nu(m')\Delta t \quad . \tag{19}$$

The first term on the rhs of eq. (19) is the probability that no jump occurred in the time interval $(0, \Delta t)$. The term $\nu(m')\Delta t$ is the probability that one jump occurred. Immediately

after such a jump, the probability density of m becomes $Q(m)$. The Focker-Planck equation for the KP reads [30,31]:

$$\frac{\partial}{\partial t}\hat{P}(m,t) = \lim_{\substack{\Delta t \to 0 \\ \Delta t \geq 0}} \{\int P_{KP}(m, \Delta t \mid m', 0)\hat{P}(m', t)dm' - \hat{P}(m,t)\}(\Delta t)^{-1} \tag{20}$$

$$= -\nu(m)\hat{P}(m,t) + Q(m)\int \nu(m')\hat{P}(m',t)dm' \quad .$$

The stationary probability density $P(m)$ of $m(t)$ is related to $Q(m)$ by :

$$Q(m) = \frac{\nu(m)P(m)}{\int \nu(m')P(m')dm'} = \frac{\nu(m)P(m)}{\langle\nu\rangle} \quad . \tag{21}$$

One can prove that for even functions $P(m)$ and $\nu(m)$, the covariance of the KP, $\tilde{\Gamma}(|t-t'|) = \langle m(t)m(t')\rangle$, is of the form [30] :

$$\tilde{\Gamma}(t) \sim \int_{\nu(0)}^{+\infty} m^2 P(m)\frac{dm}{d\nu}\exp(-\nu \mid t \mid)\, d\nu \quad . \tag{22}$$

Calculation of the frequency $\nu(m)$ requires then the inversion of the Laplace transform and the solution of a simple differential equation. In particular, for $\tilde{\Gamma}(t) = 1/t$ one obtains:

$$\nu(m) \sim \int_0^{|m|} m'^2 P(m')dm' \quad . \tag{23}$$

An important quantity is the "free path" length defined as $s = 1/\nu$. Knowing $P(m)$, we can determine the free path distribution $S(s)$ [32]. For the covariance $\tilde{\Gamma}(t) = 1/t$, this distribution can be expressed as:

$$S(s) = \frac{1}{s^2\, m^2\,(s)} \tag{24}$$

where $m(s)$ is obtained from (23). The distribution $S(s)$ decays very slowly with increasing s and the fastest rate one can obtain is $S(s) \sim s^{-2}$, in the limit of long paths.

The KP can be formulated also for higher dimensional systems. In two dimensions we have $\mathbf{m} = [m_x, m_y]$. Assuming in addition that the norm of the process is constant and equal one, $|\mathbf{m}| = 1$, the coordinates $m_x = \cos\phi$ and $m_y = \sin\phi$ and the frequency ν are

expressed in terms of a single random angle. Denoting the probability distribution of this process by $P_\Phi(\phi)$, one obtains for the covariance of the KP :

$$\tilde{\Gamma}(t) = \int_{\nu(0)}^{\infty} P_\Phi(\phi)\frac{d\phi}{d\nu}\exp(-\nu|t|)d\nu\,. \tag{25}$$

The probability distribution $P_\Phi(\phi)$ must be an even function. For $\tilde{\Gamma}(t) = 1/t$ the frequency becomes:

$$\nu(\phi) = \int_0^{\phi} P_\Phi(\phi')d\phi' \tag{26}$$

and the free path distribution $S(s)$ appears to be independent of $P_\Phi(\phi)$ and takes the simple form:

$$S(s) \sim s^{-2}\,. \tag{27}$$

According to (26), the free path becomes infinite for $\phi = 0$.

The KP can be also applied to generate a stochastic process with another kind of auto-correlation function, in particular an arbitrary algebraic covariance $\tilde{\Gamma}(t) \sim |t|^{-1/\kappa}$ $(\kappa > 0)$. In two dimensions, the frequency ν of that process becomes:

$$\nu = \left(\int_0^{\phi} P_\Phi(\phi')d\phi'\right)^{\kappa}, \tag{28}$$

implying the free path distribution $S(s) \sim s^{-(1+\frac{1}{\kappa})}$. Technically, one can then generate the stochastic process with covariance (10) in the following way:

i) Choose a random number ϕ, uniformly distributed in the interval $(0, 1)$,

ii) Calculate $m_x = \sqrt{\alpha}\cos\phi/\sqrt{\epsilon}$ and $m_y = \sqrt{\alpha}\sin\phi/\sqrt{\epsilon}$,

iii) Choose signs of m_x and m_y, independently and with equal probability,

iv) Determine the time interval $\Delta t = \epsilon/\phi$ within which the process keeps the value (m_x, m_y).

The described procedure assumes a uniform probability $P_\Phi(\phi)$ and does not care about the angular distributions. In fact, this particular process is non-isotropic. If a physical problem imposes specific requirements concerning angular symmetry, the algorithm can easily be modified [32].

The covariance does not determine a stochastic process completely and some properties of GLE solutions, with the KP as the stochastic force, must be sensitive to higher-order autocorrelations. However, the VAF and the transport properties implied by it, depend only on the covariance C_F.

IV. THE NUMERICAL RESULTS FOR V(R)=0

The two-dimensional KP described in Sec.III will serve to realize the stochastic force in the generalized Langevin problem. Thus we have:

$$\mathbf{F}(t) = \mathbf{m}(t) \,. \tag{29}$$

The autocorrelation function of this force is given by (10). The average is taken over a statistical ensemble which is defined by the uniform probability density distribution $P_\Phi(\phi)$. The parameter ϵ has a simple interpretation, namely it is equal to the shortest time step within which the force is constant.

The force (29) is an integrable function. Obviously, it fulfills the condition (4). The most distinctive feature of $\mathbf{F}(t)$ is the presence of long periods of time when its value remains constant. Those intervals are interwoven with regions of rapid change as can be seen in Fig. 2 which shows the running sum of one component of the stochastic force as a function of time. Due to the scale invariance of the free path distribution $S(s)$, the plot is self-similar, i.e. a magnification of any of its part including rapid variations, gives statistically the same sequence of long and short intervals. This magnification procedure has its limit at the interval scale ϵ.

We solve now the equation (3) with $V(\mathbf{r}) = 0$ and the initial conditions:

$$\mathbf{v}(0) = \mathbf{r}(0) = 0 \,. \tag{30}$$

Since the kernel $K(t-\tau)$ depends only on time differences, the equation can be solved using the Laplace transform technique [33] . We have found the following solution, valid under the assumption that $\mathbf{v}(t)$ does not change substantially within the interval of size ϵ:

$$\mathbf{v}(t) = \mathbf{g}(t) + \int_0^t R(t-\tau)\,\mathbf{g}(\tau)\,d\tau \tag{31}$$

and

$$\mathbf{r}(t) = \mathbf{h}(t) + \int_0^t R(t-\tau)\,\mathbf{h}(\tau)\,d\tau \tag{32}$$

where

$$\begin{aligned} \mathbf{g}(t) &= m^{-1}\int_0^t \mathbf{F}(\tau)\,d\tau \\ \mathbf{h}(t) &= \int_0^t \mathbf{g}(\tau)\,d\tau\ . \end{aligned} \tag{33}$$

The resolvent $R(t)$ is given as the inverted Laplace transform of the following function:

$$\tilde{R}(s) = \frac{\alpha\,(\mathrm{E}i(-\epsilon s) - 1)}{mTs + \alpha\,(1 - \mathrm{E}i(-\epsilon s))}\,. \tag{34}$$

One can easily check that $R(t)$ is related to the time-derivative of the function χ (15):

$$R(t) = \frac{d}{dt}\chi\,(t) \qquad (t > 0)\ . \tag{35}$$

The functions $\mathbf{g}(t)$ and $\mathbf{h}(t)$ are continuous and single-valued for all $t \geq 0$. Thus the integrals in (31) and (32) can be understood in standard Riemannian sense. Fig. 3 shows an exemplary trajectory in both the velocity space and the configuration space. The intermittent structure of long and short intervals of noise variations is visible also here, exhibiting a picture typical for Lévy walks [34]. The plotted trajectories, especially $\mathbf{r}(t)$, are relatively smooth functions. Despite the fact that the driving force assumes both positive and negative values with equal probability, the trajectory $\mathbf{r}(t)$ departs continuously from the origin and the reflection symmetry is apparently broken.

Using (31), we can calculate directly the second moment of the velocity distribution, $\langle \mathbf{v}^2 \rangle(t)$. The averaging is performed according to the procedure explained in Sec.III, i.e. over a statistical ensemble constructed by a uniform sampling of the noise direction ϕ. We have calculated trajectories in the velocity space up to a given time t , according to (31) and with the initial conditions (30). Then the average of $\langle \mathbf{v}^2 \rangle(t)$ has been taken. Fig. 4

presents the results for $\epsilon = 10^{-2}$ and $T = 1$. Clearly, the velocity variance does not reach any equilibrium. It stabilizes for a while but then grows again. The second moment is thus divergent as one could expect for Lévy flights [2] and the parameter T can no longer be identified with the temperature. The entire velocity distribution does expand with time. Fig. 5 presents the distribution of $\mathbf{v}^2$. It broadens with time and the shape of the distribution indicates the presence of long flights in the form of a peak which becomes diffused at longer times. On the right hand side of the peak, at high energies, another structure develops which results from the gradual equilibrization. This structure tends asymptotically to the Maxwellian distribution.

Similarly, one can obtain from (31) the VAF $\langle \mathbf{v}(t_0)\mathbf{v}(t) \rangle$. Fig. 6 presents the result of numerical calculation for $t_0 = 3$. The chosen set of parameters corresponds to the case which is shown in Fig. 1 by the solid line. The present result does not exhibit any negative tail. The VAF falls rapidly for t close to t_0, similarly as in Fig. 1, but then oscillates around a stabilized value $C_\infty = 0.33$. Knowing the asymptotic behaviour of $C(t)$ one can assess the rate of diffusion by means of (17). In contrast to the results of Sec.II, the diffusion appears strongly enhanced: $\langle \mathbf{r}^2 \rangle = C_\infty t^2$, and the diffusion coefficient grows lineary with time, as for the ballistic motion. This outcome can be confirmed by direct evaluation of the mean squared displacement $\langle \mathbf{r}^2 \rangle$, using (32). We have indeed found the quadratic time-dependence for $\langle \mathbf{r}^2 \rangle$, as Fig. 7 shows. Moreover, the parabola parameter approximately equals C_∞.

The rapid, ballistic diffusion rate results from the existence of long periods of constant noise values and is related to statistics of the free paths. Zumofen and Klafter [4] have shown, studying a simple map, that the free path distribution (27) implies a slightly slower growth of the mean square displacement: $\langle \mathbf{r}^2 \rangle \sim t^2/\log t$. However, such time dependence cannot be excluded also in our case because the logarithmic modification is weak and may easily be overlooked in numerical calculations.

A similar observation has been made in the recent study of diffusion in the Knudsen gas [35] , where for a large variety of the algebraic chord length distributions running at large distances, the Knudsen diffusion is a Lévy walk which is dominated by the ballistic

dynamics.

V. THE BROWNIAN OSCILLATOR – THE ESCAPE FROM THE POTENTIAL WELL

So far we have discussed the motion of particle subjected only to the stochastic force and retarded friction. Now we add the harmonic oscillator potential:

$$V(\mathbf{r}) = \omega \mathbf{r}^2/2 \tag{36}$$

and solve the GLE (3) with the noise correlations (10) and the initial conditions (30). Applying the same procedure as in Sec.IV, we find the solution also in the form (31) and (32). The Laplace transform of the resolvent is now given by :

$$\tilde{R}(s) = \frac{\alpha\,(\mathrm{E}i(-\epsilon s) - 1)/mT - \omega/s}{s + \alpha\,(1 - \mathrm{E}i(-\epsilon s))/mT + \omega/s} \tag{37}$$

The resolvent itself, $R(t) = \mathcal{L}^{-1}[\tilde{R}(s)]$, becomes:

$$\begin{aligned} R(t) &= \mathrm{e}^{-at}\,(c_1 \sin bt + c_2 \cos bt) + \\ &+ mT/\alpha \int_0^\infty \frac{x\,\mathrm{e}^{-tx}\,dx}{(mTx/\alpha + \mathrm{E}i_1(\epsilon x) - 1 + mT\omega/\alpha x)^2 + \pi^2} \quad . \end{aligned} \tag{38}$$

An important application of the above formalism is a study of the particle escape from a spherically symmetric potential well. Let us assume that the particle rests initially at the bottom of the well (36) and its motion is governed by (3). The stochastic force $\mathbf{F}(t)$ accelerates the particle which may eventually reach the top of the well at $|\mathbf{r}| = r_B$. At this time, all interactions: the potential, the stochastic force and the friction, are switched off and the particle escapes freely. Thus we shall study the generalized Langevin problem with an absorbing barrier. Physically, one can model in this way the evaporation process. A quantity of interest, accessible experimentally, is the distribution of total energy of escaping particles, $P(E)$. In order to derive this distribution from the GLE, one should know the

velocity at $|\mathbf{r}| = r_B$. Technically, the particle position $\mathbf{r}(t)$ has been calculated from (32). The inverse of this function at $|\mathbf{r}| = r_B$, determines the time when the barrier is reached. In turn, (31) for $t = t(r_B)$ gives the velocity $\mathbf{v}_B$ at the barrier. The final, asymptotic energy is $E = \omega r_B^2/2 + m\mathbf{v}_B{}^2/2$.

The energy distribution of escaping particles is shown in Fig. 8. The parameters, $T = 100$, $\epsilon = 10^{-2}$, $m = 1$, $r_B = 50$ and $\omega = 0.032$, have been chosen to allow comparison with solutions of the ordinary Langevin equation (1) [11,32]. Those results, obtained from (1), have two characteristic features: (i) the peak at relatively low energies and (ii) the Gaussian tail. The peak may be interpreted as a manifestation of long free paths and attributed to particles escaping due to long-time action of a constant stochastic force, i.e. without any randomization. The Gaussian tail, in turn, results from particles subjected to only limited number of noise variations, which is not enough to attain the equilibrium state. The GLE produces a similar peak (shown in Fig. 8) but its form is more diffused and dominates the entire spectrum. The right flank falls very slowly, like a power law, and then bends down, reflecting the similar trend for the potential-free case (see Fig. 5).

Fig. 9 shows the survival probability for particles inside the wall, defined as a number of particles which yet have not leave the well at a time t. This probability is exponential, in a sharp contrast with the standard Langevin equation, always predicting the tail $1/t$ [36].

One could argue that the outcome concerning energy distributions must be of minor physical significance if the system does not possess a stable velocity distribution and the average energy diverges with the time. However, it is not the case in the high T limit. For large values of T , Fig. 10 presents the time dependence of the velocity variance of Brownian particle subjected to the harmonic oscillator force, without absorbing barrier. Now $\langle \mathbf{v}^2 \rangle(t)$ reaches a stationary value. Moreover, this stationary value is proportional to the parameter T which, in turn, can now be identified with the temperature of the equilibrium state. Thus in the high-T limit, the dissipation-fluctuation theorem (8) holds.

VI. SUMMARY AND CONCLUSIONS

The Langevin equation with strongly correlated stochastic force reveals phenomena unknown to the standard Brownian motion theory which assumes either white or coloured (exponential) noise. Proper handling of the friction force leads to the generalized, integro-differential equation, including the memory kernel. In the present paper we have solved this equation assuming the noise autocorrelation function with the tail which is proportional to $1/t$. Usually, one postulates that the Brownian particle, described by the GLE, is in the equilibrium with a heat bath of given temperature. Then its velocity and position probability distributions are stationary and stable with finite moments and the velocity autocorrelation function can be easily derived. In the case of the $1/t$ noise correlations , the VAF has the algebraic tail and is negative value for large t . Nevertheless, the integral of the VAP, i.e. the diffusion coefficient, is finite and the GLE does not predict any kind of the anomalous diffusion. Thus the transport properties of the system, as determined by the VAF, do not differ substantially from those for rapidly falling noise correlations.

On the other hand, one can directly calculate the VAF and the diffusion rate by simulating the stochastic force numerically. For that purpose, the kangaroo process has been applied. The tail of the VAF oscillates now around a constant, finite value, rendering that the diffusion rate is ballistic, i.e. $\langle \mathbf{r}^2 \rangle \sim t^2$. This system is unable to reach any equilibrium state because the second moment of the velocity distribution $\langle \mathbf{v}^2 \rangle$, diverges with time. Also the energy distribution broadens constantly. It consist of two parts: a peak, connected with long paths of Brownian particle subjected to a constant acceleration, and the Maxwellian tail. The divergent moments are characteristic for Lévy flights. Numerically simulated trajectories, both in the velocity space and in the configurational space, are typical for intermittent structure of Lévy flights: long regular segments are separated by points of rapid direction change and outbursts of irregular motion. In this way, solutions of the GLE reflect properties of the KP which can go through very long paths: the free paths distribution for KP falls off like $1/s^2$. Despite irregularities, trajectories in the configurational space are

relatively smooth, having a continuous first derivative.

It is probably useful at this moment to mention that the Knudsen diffusion in three-dimensional for the algebraic pore chord distribution $\zeta(r) \sim 1/r^{\mu^*}$ and $1 < \mu^* < 2$ is the Lévy walk dominated by the ballistic dynamics, similarly as found in this work. This is an important analogy in view of the significance of the Knudsen gas concept for a phenomenological description of the nuclear one-body dissipation [37] , which is a dominant dissipation mechanism at low excitation energies. Hence, the GLE with the correlated stochastic force could be a microscopic generalization of the phenomenologically successful nuclear one-body dissipation mechanism.

Usually, the memory kernel is taken as proportional to the noise autocorrelation function in order to satisfy the dissipation-fluctuation theorem. In general, this assumption is not sufficient for that purpose because the equilibrium state is not reached and, hence, the temperature is not determined. However, as we have shown in the case of the harmonic oscillator potential, the equilibrium state is restored in the high-T limit. This conclusion has important consequences for possible applications because the divergent moments are usually non-physical. Indeed, it is so, e.g., for the evaporation process. We have modelled this process assuming the potential well in the form of the harmonic oscillator and looking for the solution of a problem with the absorbing barrier. The shape of the energy distribution of the escaping particles is dominated by a wide peak with slowly falling right flank. A more rapid fall shows up only at very high energies and corresponds to a very small probability.

The comparison of results of the present paper with Ref. [11] allows to assess the influence of memory effects on calculated quantities. There are some similarities, e.g., the velocity (energy) spectra for both approaches possess the peak attributed to long intervals of constant value of the stochastic force. However, its shape is different: the tail of the energy distribution of particles escaping from the potential well for the Markovian, memory-free case is Gaussian, independently of the noise generator used [32]. The survival probability also changes. Introducing the retarded friction changes its shape from the algebraic one, proportional to $1/t$, into the exponential one. This modification of the survival probability

tail brings about a qualitative change: the average time the particle spends inside the well, $\bar{t} \sim \int_0^\infty tN(t)dt$, becomes finite. Last but not least, in contrast to the results obtained using the GLE, the memory-free Langevin equation *always* implies the full equilibrization though not in accordance with the fluctuation-dissipation theorem.

The regularization of the force autocorrelation function $1/t$ near $t = 0$, in the form (10), is necessary to avoid a singularity which would result in a trivial solution $\mathbf{v}(t) \equiv 0$ if $\epsilon \to 0$. What is then the meaning and importance of the parameter ϵ? Numerical results are not very sensitive on it since ϵ enters formulas only logarithmically. Fig. 1 can serve as an illustration. The parameter ϵ influences the rate of change of the noise, namely, the smallest time step of the noise variation is just ϵ. As we have mentioned in the Introduction, the stochastic force with the covariance proportional to $1/t$ can be generated also by means of a non-Markovian, deterministic system – the periodic Lorentz gas, equivalent to the generalized Sinai billiard. The Lorentz gas applies as a useful model of physical processes, e.g. in hydrodynamics. According to that picture, ϵ corresponds to the smallest path the particle can experience between subsequent collisions with scatterers and depends on the geometry of billiard. Consequently, the practical choice of a value of ϵ for a particular physical problem should stem from origin and interpretation of the stochastic force.

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APPENDIX

The Appendix is devoted to the derivation of integral (13). We choose the contour $\mathcal{C}$ comprising a straight line parallel to the imaginary axis, positioned at any positive σ, and the large half-circle in the left half-plane. The plane is cut along the negative real axis. The integral over the half-circle vanishes from the Jordan lemma for $t > 0$. Thus we have: $\frac{1}{2\pi i}\int_{\mathcal{C}} = \frac{1}{2\pi i}\int_{-\infty+\sigma}^{\infty+\sigma} + \frac{1}{2\pi i}(\int_{-\infty+i0}^{0+i0} - \int_{-\infty-i0}^{0-i0}) \equiv C(t) - I = S$ where S denotes the sum over residues. The integrand possesses two conjugate simple poles at $z_{1,2} = -a \pm bi \quad (a > 0)$. The singular points can easily be found numerically using the following expansion:

$$\mathrm{E}i(z) = \gamma + \ln(-z) + \sum_{n=1}^{\infty}(-z)^n/n!\,n. \tag{39}$$

After some algebra, we obtain:

$$S = T^2/\alpha \left(\frac{\exp(z_1 t)}{mT/\alpha + \epsilon - 1/z_1 + O(\epsilon^2)} + c.c.\right) = \mathrm{e}^{-at}(c_1 \sin bt + c_2 \cos bt) \tag{40}$$

where $c.c.$ means the complex conjugate. The constants are given by: $c_1 = bA$, $c_2 = [(mT/\alpha + \epsilon)(a^2 + b^2) + a]\,A$ and

$$A = \frac{2mT/\alpha}{(mT/\alpha + \epsilon)^2(a^2 + b^2) + 2a(mT/\alpha + \epsilon) + 1}\,.$$

To calculate the sum of integrals I we utilize the following property of the integral exponent: $\mathrm{E}i(x \pm i0) = \mathrm{E}i_1 x \mp \pi i \quad (x > 0)$. Combining the results for S and I, we get (14).

REFERENCES

[1] P. Hänggi and P. Jung, Adv. Chem. Phys. **89**, 229 (1995).

[2] J. Klafter and G. Zumofen, Phys. Rev. **E49**, 4873 (1994).

[3] T. Geisel, A. Zacherl and G. Radons, Z. Phys. B **B71**, 117 (1988).

[4] G. Zumofen and J. Klafter, Physica **D69**, 436 (1993).

[5] R. F. Grote and J. T. Hynes, J. Chem. Phys. **73**, 2715 (1980).

[6] P. Hänggi, J. Stat. Phys. **30**, 401 (1983).

[7] A. Igarashi and T. Munakata, J. Phys. Soc. Jpn. **57**, 2439 (1988).

[8] A. Brissaud and U. Frisch, J. Quant. Spectrosc. Radiat. Transfer **11**, 1767 (1971).

[9] T. Srokowski and M. Płoszajczak, Phys. Rev. Lett. **75**, 209 (1995).

[10] S. Drożdż, J. Okołowicz, M. Płoszajczak and T. Srokowski, Preprint GANIL P 96 09.

S. Drożdż, J. Okołowicz, M. Płoszajczak and T. Srokowski, *Fractal Frontiers*, M. M. Novak and T. G. Devey eds., (World Scientific, 1997), p.141-150.

[11] M. Płoszajczak and T. Srokowski, Ann. Phys. (N.Y.) **249**, 236 (1996).

[12] H. Mori, Prog. Theor. Phys. **33**, 423 (1965).

[13] R. Kubo, Rep. Prog. Phys. **29**, 255 (1966).

[14] J. Boussinesq, *Théorie analitique de la chaleur*, II (Gauthiers-Villars, Paris, 1903).

[15] P. Hänggi, P. Talker and M. Borkovec, Rev. Mod. Phys. **62**, 251 (1990).

[16] H.A. Kramers, Physica **7**, 284 (1940).

[17] S. K. Sarker, J. H. Davies, F. S. Khan and J. W. Wilkins, Phys. Rev. **B33**, 7263 (1986).

[18] K. Morawetz, R. Walke and G. Roepke, Phys. Lett. **A190**, 96 (1994).

[19] D. B. T. Thoai and H. Haug, Z. Phys. **B91**, 199 (1993).

[20] S. Ayik, Z. Phys. **A350**, 45 (1994).

[21] Y. Abe, S. Ayik, P.-G. Reinhard and E. Suraud, Phys. Rep. **275**, 49 (1996).

[22] B. J. Alder and T. E. Wainwright, Phys. Rev. **A1**, 18 (1970).

[23] R. M. Mazo, J. Chem. Phys. **54**, 3712 (1971).

[24] B. Cichocki and B. U. Felderhof, J. Stat. Phys. **87**, 989 (1997).

[25] B. U. Felderhof, J. Phys. A: Math. Gen. **11**, 921 (1978).

[26] B. J. Berne and G. D. Harp, Adv. Chem. Phys. **17**, 63 (1970).

[27] T. S. Chow and J. J. Hermans, J. Chem. Phys. **56**, 3150 (1972).

[28] B. J. Alder, in *Molecular-dynamics simulation of statistical-mechanical systems*, (North-Holland, Amsterdam, 1986), p.66.

[29] A. Rahman, Phys. Rev. **A2**, 405 (1964).

[30] A. Brissaud and U. Frisch, J. Math. Phys. **15**, 524 (1974).

[31] A.T. Bharucha-Reid, *Elements of the Theory of Markov Processes and Their Applications* (McGraw & Hill, New York, 1960).

[32] M. Płoszajczak and T. Srokowski, Phys. Rev. **E55**, 5126 (1997).

[33] V.I. Smirnov, *The course of higher mathematics*, Vol. 4 (Russian edition, Moskva 1951).

[34] J. Klafter, M. F. Shlesinger and G. Zumofen, Physics Today, 33 (February 1996).

[35] P. Levitz, *From Knudsen diffusion to Levy walks*, Preprint CRMD/Orleans (1997).

[36] By mistake, the case supposed to be marked by solid line in Fig. 2 of Ref. [32] has not appeared in the plot. This line has the shape $1/t$.

[37] J. Błocki, Y. Boneh, J.R. Nix, J. Randrup, M. Robel, A.J. Sierk and W.J. Swiatecki, Ann. Phys. (N.Y.) **113**, 330 (1978).

Figure captions

Fig. 1

The velocity autocorrelation function calculated from (14) for $\epsilon = 10^{-2}$ with $T = 1$ (the solid line) and $T = 0.5$ (the long-dashed line). The short-dashed line corresponds to $\epsilon = 5 \cdot 10^{-3}$ and $T = 1$. The particle mass is $m = 1$. The negative tail is algebraic with an universal exponent equal -1.18 .

Fig. 2

The running sum $S_F(t) \equiv \sum_i F_i$, where $F_i = F(t')$ in the time interval $t'_i \leq t' < t'_{i+1}$, are subsequent constant values of one component of the stochastic force generated by the two-dimensional KP and $\epsilon = 0.01$. Since a term is added to the sum only when the force assumes a new value, S_F remains constant between subsequent changes of the force change. The sum comprises 300 terms for $t = 20$.

Fig. 3

A particle trajectory in the velocity (left side) and in the configuration (right side) spaces for $\epsilon = 10^{-2}$ and $T = 1$. The particle mass is $m = 1$. Both pictures correspond to the time interval $t \in (0, 20)$. The initial conditions are given by (30).

Fig. 4

The variance of the velocity distribution $\langle \mathbf{v}^2 \rangle$ as a function of time for $\epsilon = 10^{-2}$ and $T = 1$.

Fig. 5

The time evolution of the distribution $P(\mathbf{v}^2)$ for $\epsilon = 10^{-2}$ and $T = 1$. The curves corresponds to the following times: $t = 5$ (solid line), $t = 20$ (dots) and $t = 50$ (triangles). All distributions are normalized to unity.

Fig. 6

The velocity autocorrelation function $C(t) = \langle \mathbf{v}(t_0)\mathbf{v}(t) \rangle$ where $t_0 = 3$, for $\epsilon = 10^{-2}$ and $T = 1$.

Fig. 7

The mean square displacement $\langle \mathbf{r}^2 \rangle$ as a function of time for $\epsilon = 10^{-2}$ and $T = 1$.

Fig. 8

The energy distribution of particles escaping from the harmonic oscillator potential well (36) which is cut at $|\mathbf{r}| = r_B$. The parameter values are: $T = 100$, $\epsilon = 10^{-2}$, $m = 1$, $r_B = 50$ and $\omega = 0.032$. The statistical ensemble consist of 50000 trajectories. The distribution is normalized to unity.

Fig. 9

The number of trajectories which do not escape from the potential well (36) up to the time t (the survival probability). The parameters are the same as in Fig. 8.

Fig. 10

The variance of the velocity distribution $\langle \mathbf{v}^2 \rangle$ as a function of time for a particle in the harmonic oscillator potential (36). The solid line corresponds to $T = 100$ and the dashed line to $T = 50$. The other parameters are the same as in Fig. 8. The averages were taken over 5000 trajectories for each point.

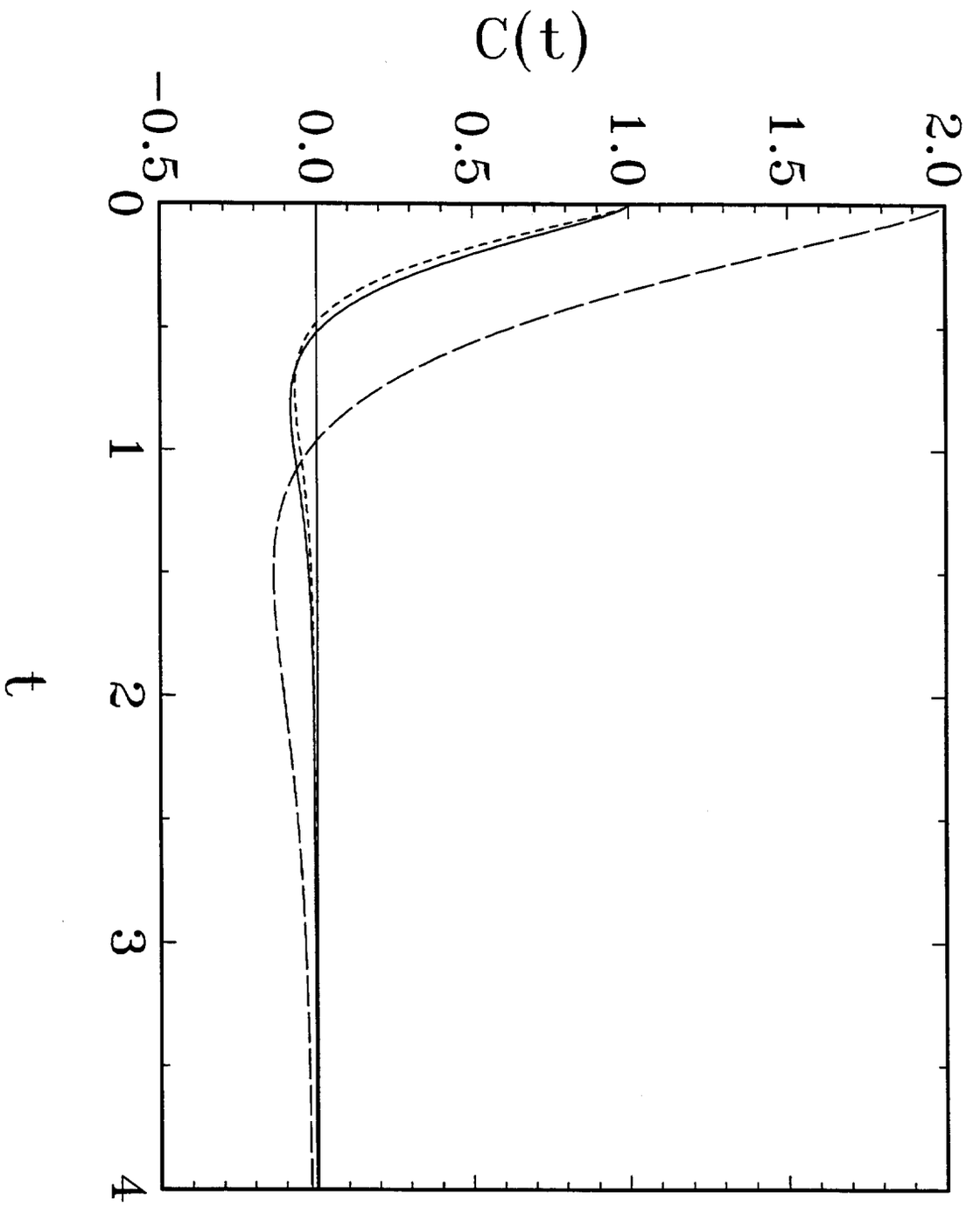


Fig. 1

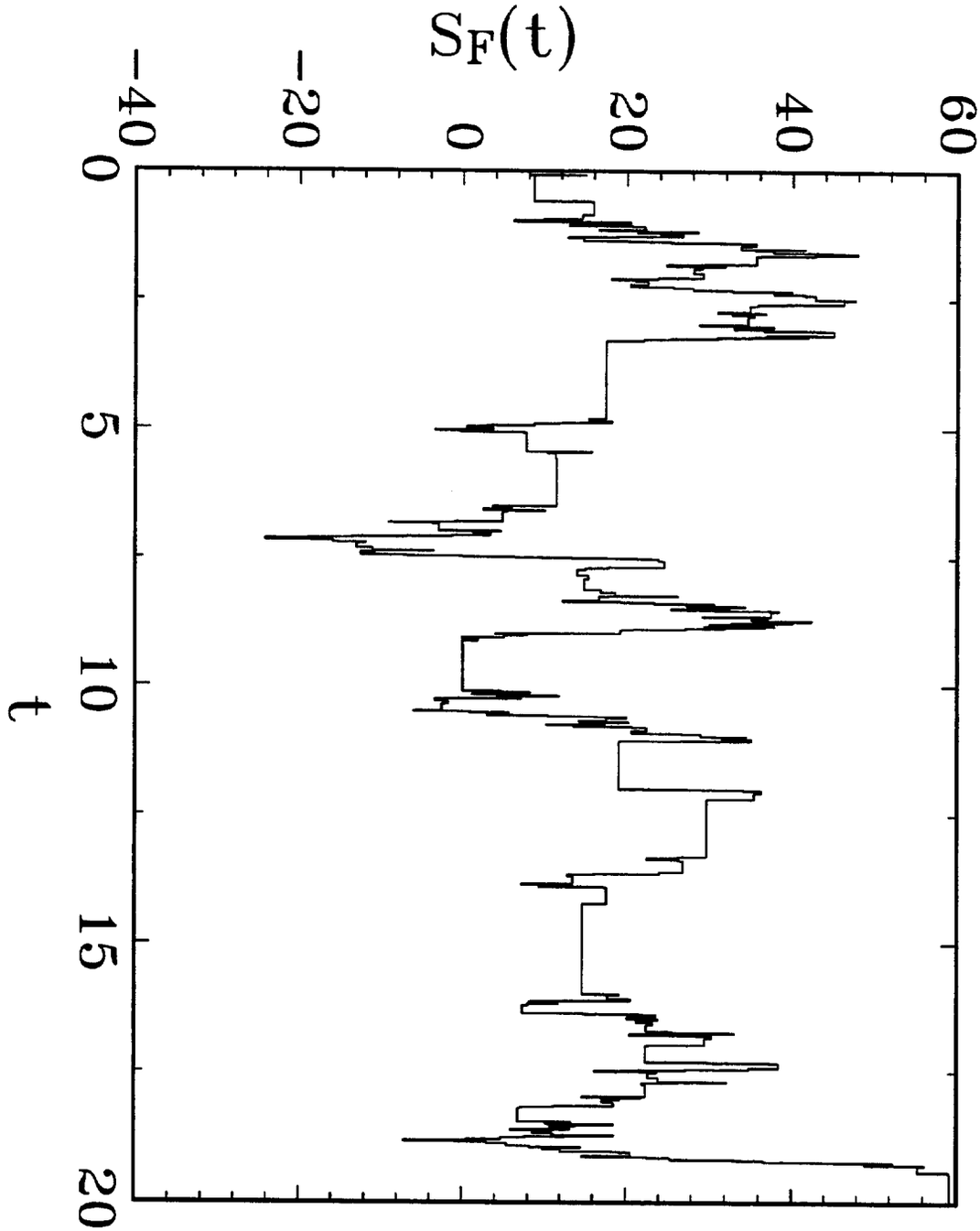


Fig. 2

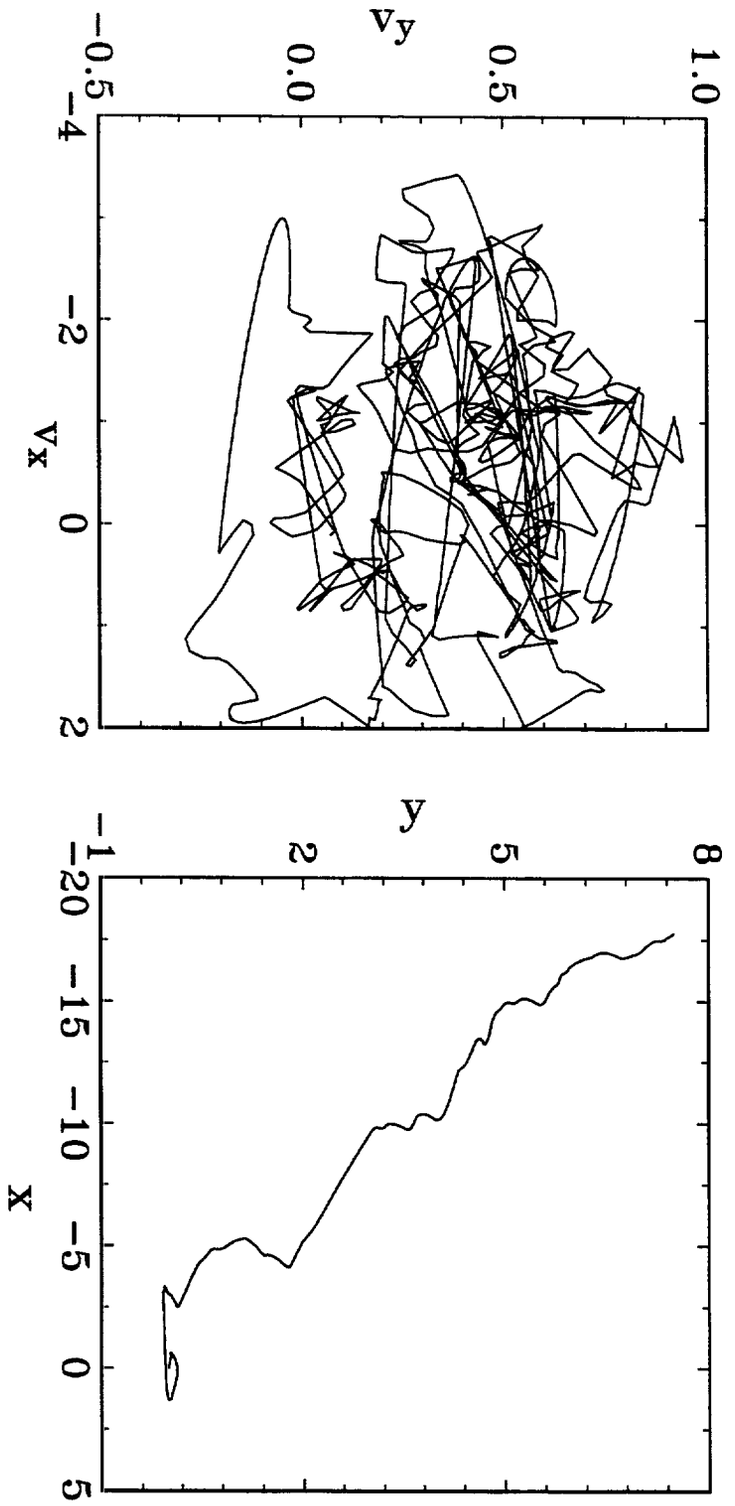
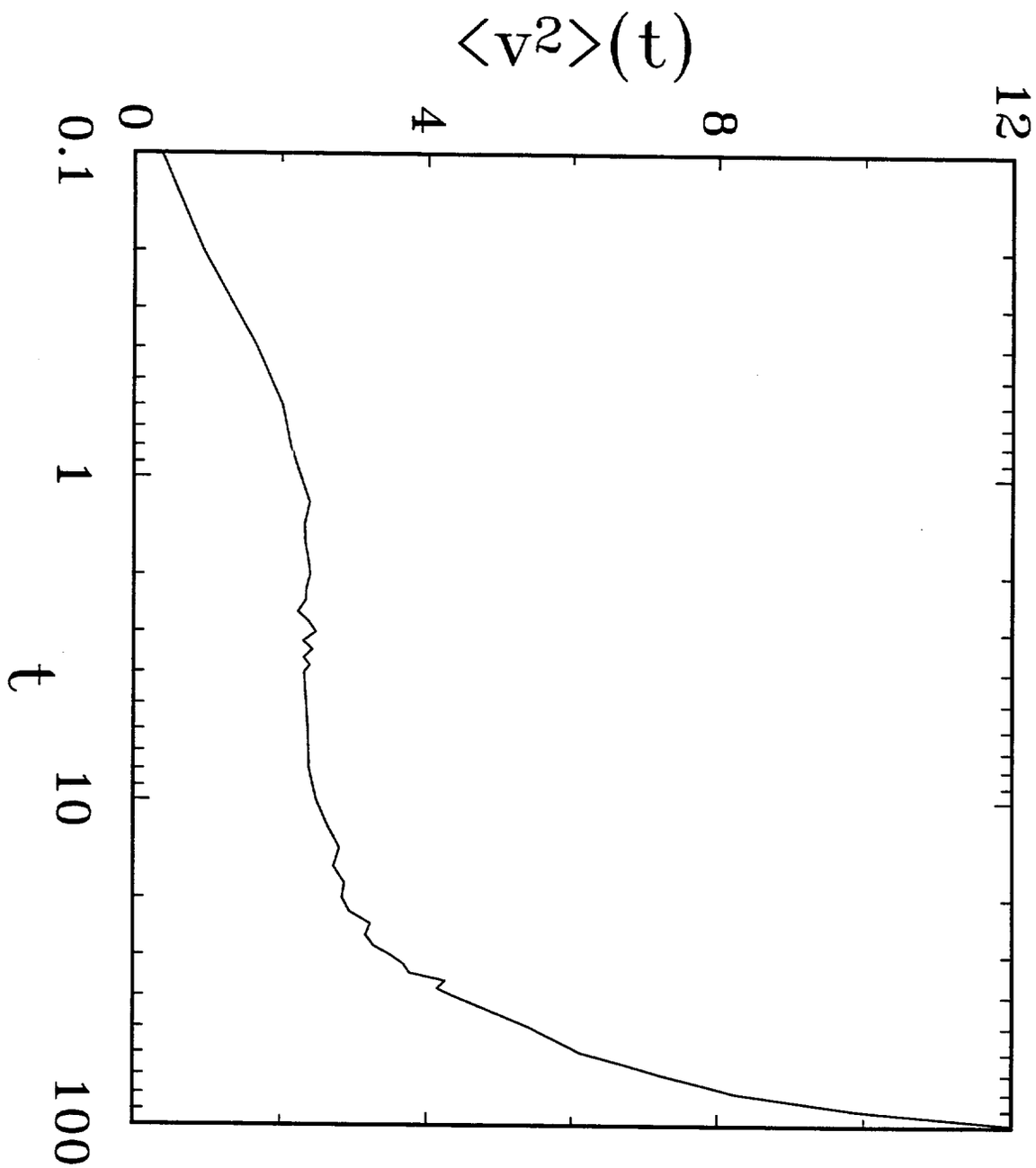


Fig. 3



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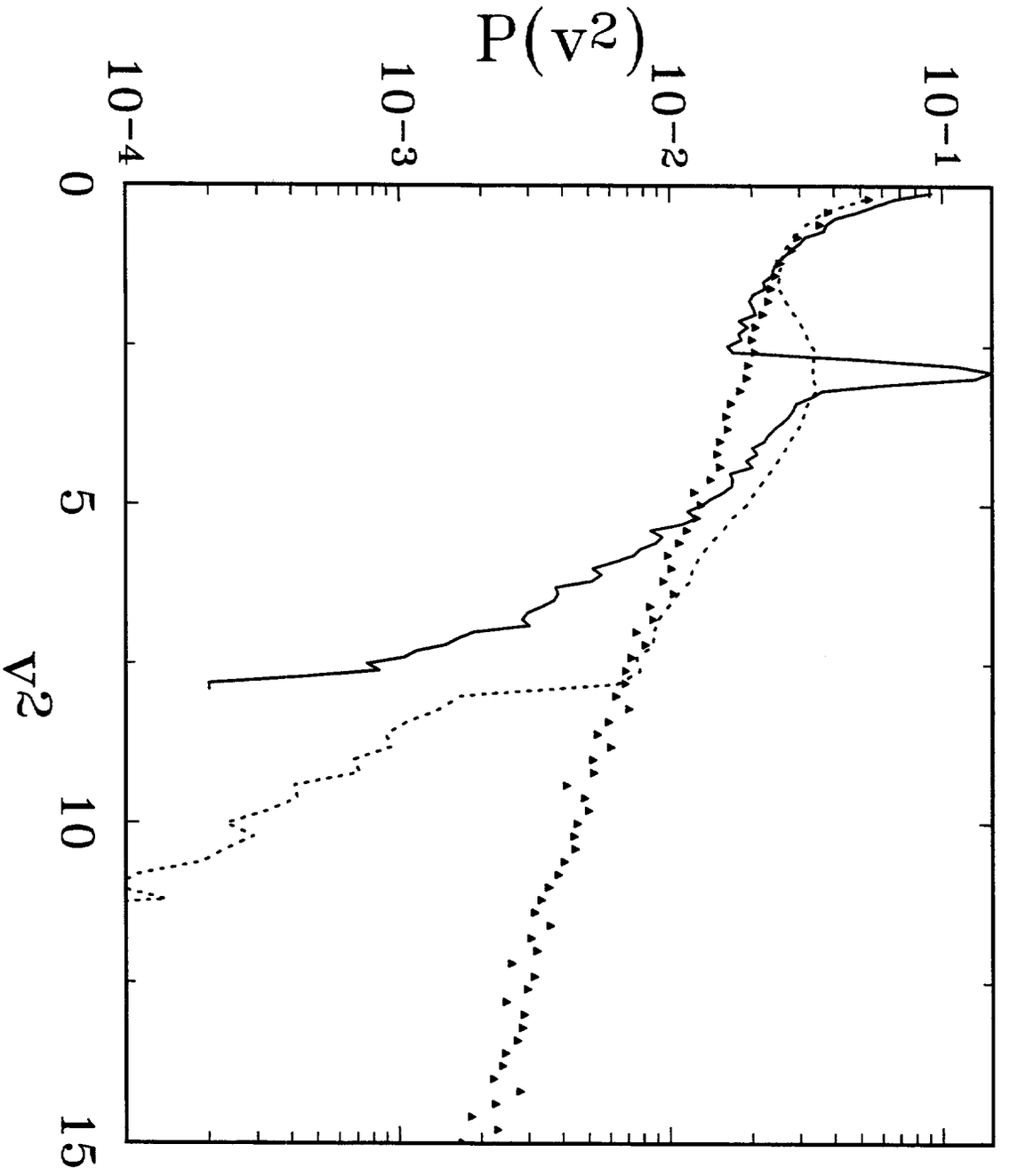

Fig. 5

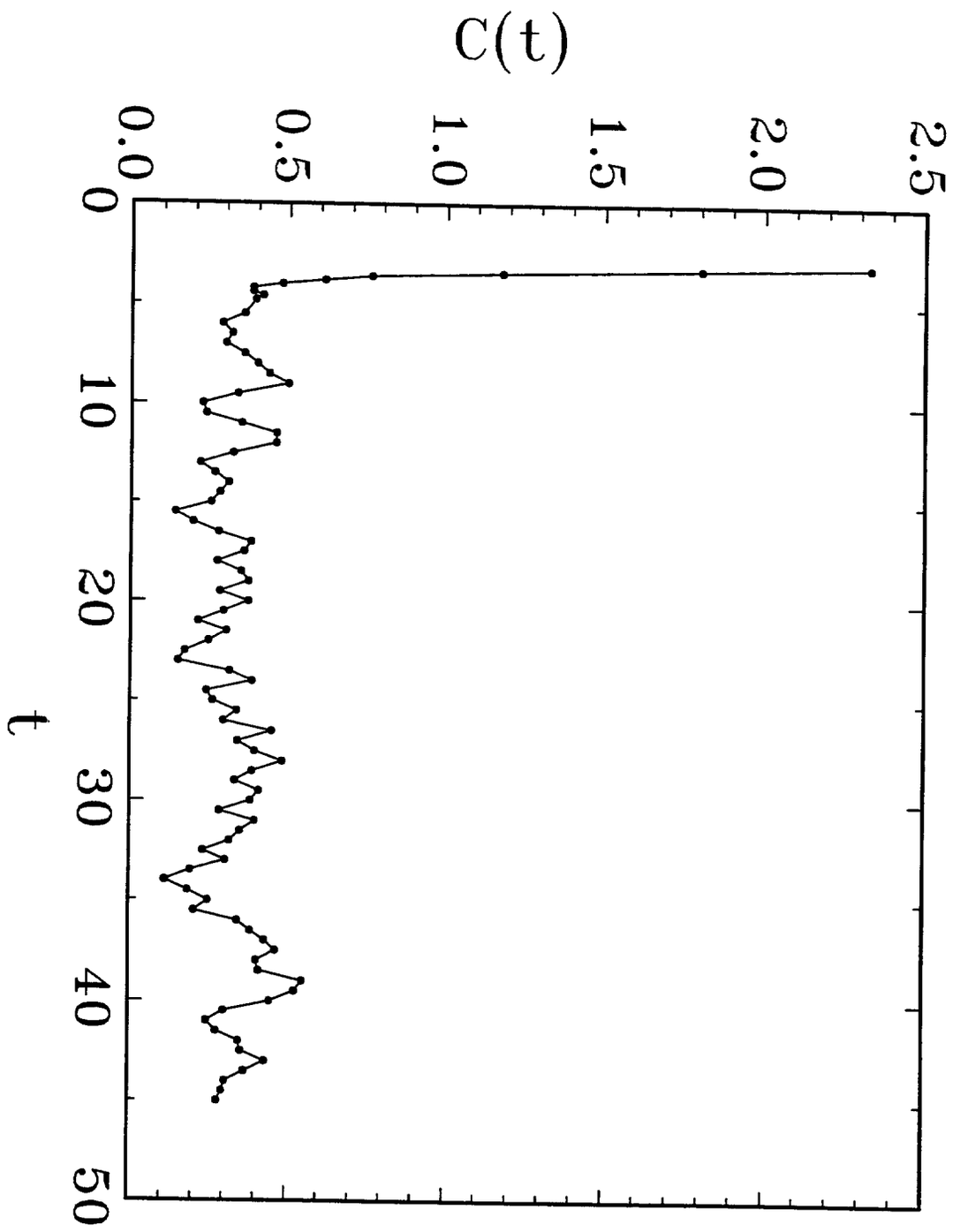

Fig. 6

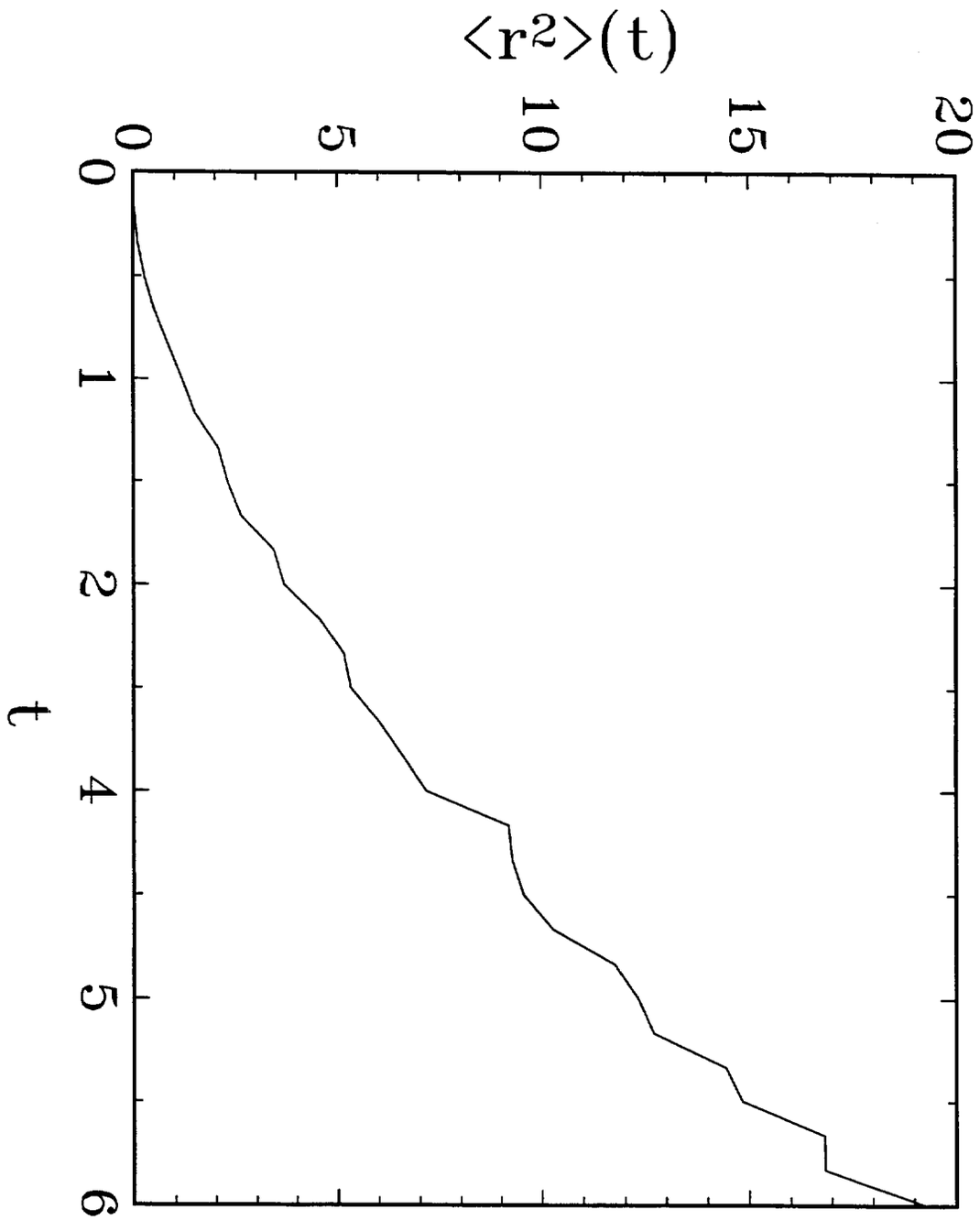

Fig. 7

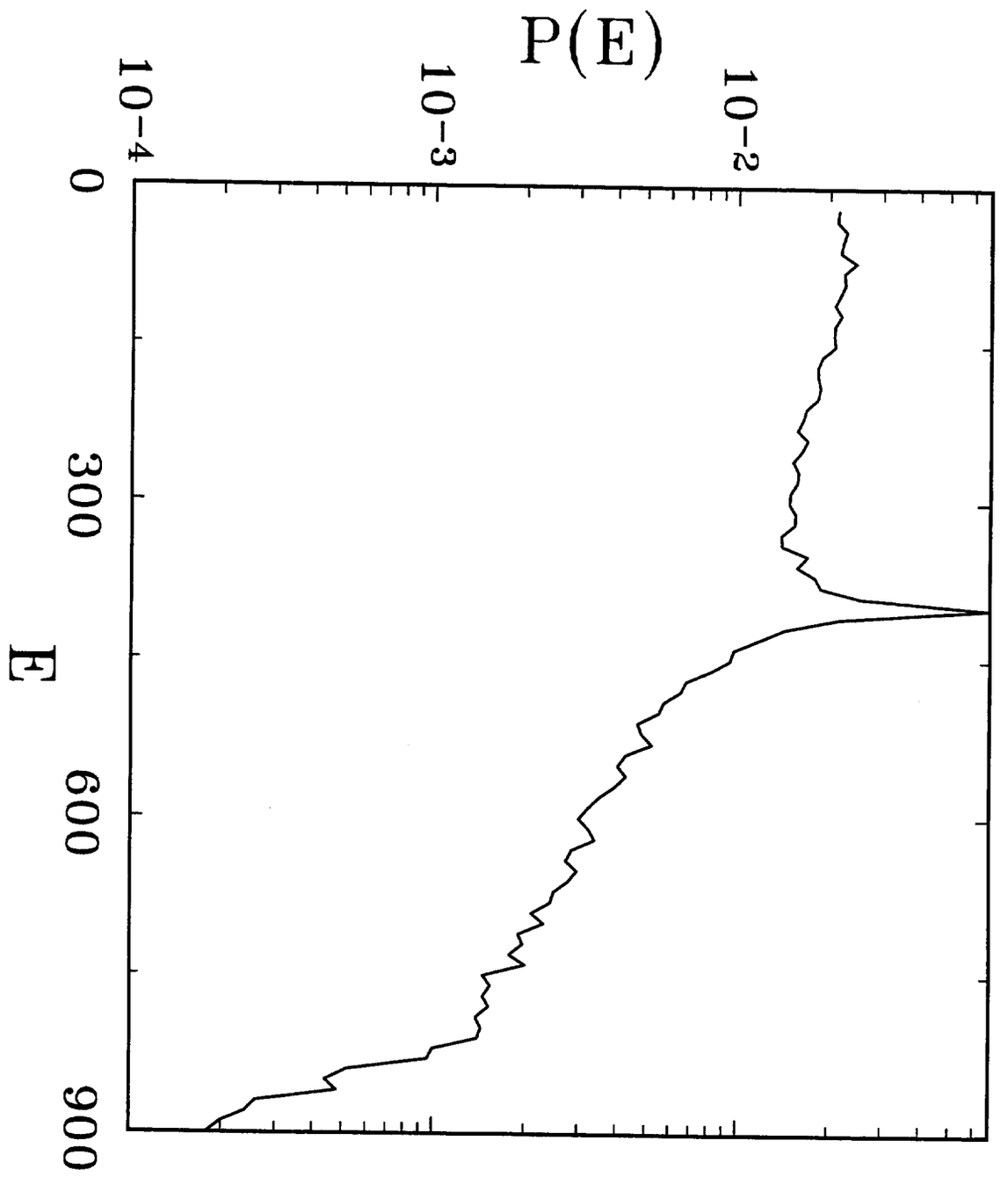

Fig. 8

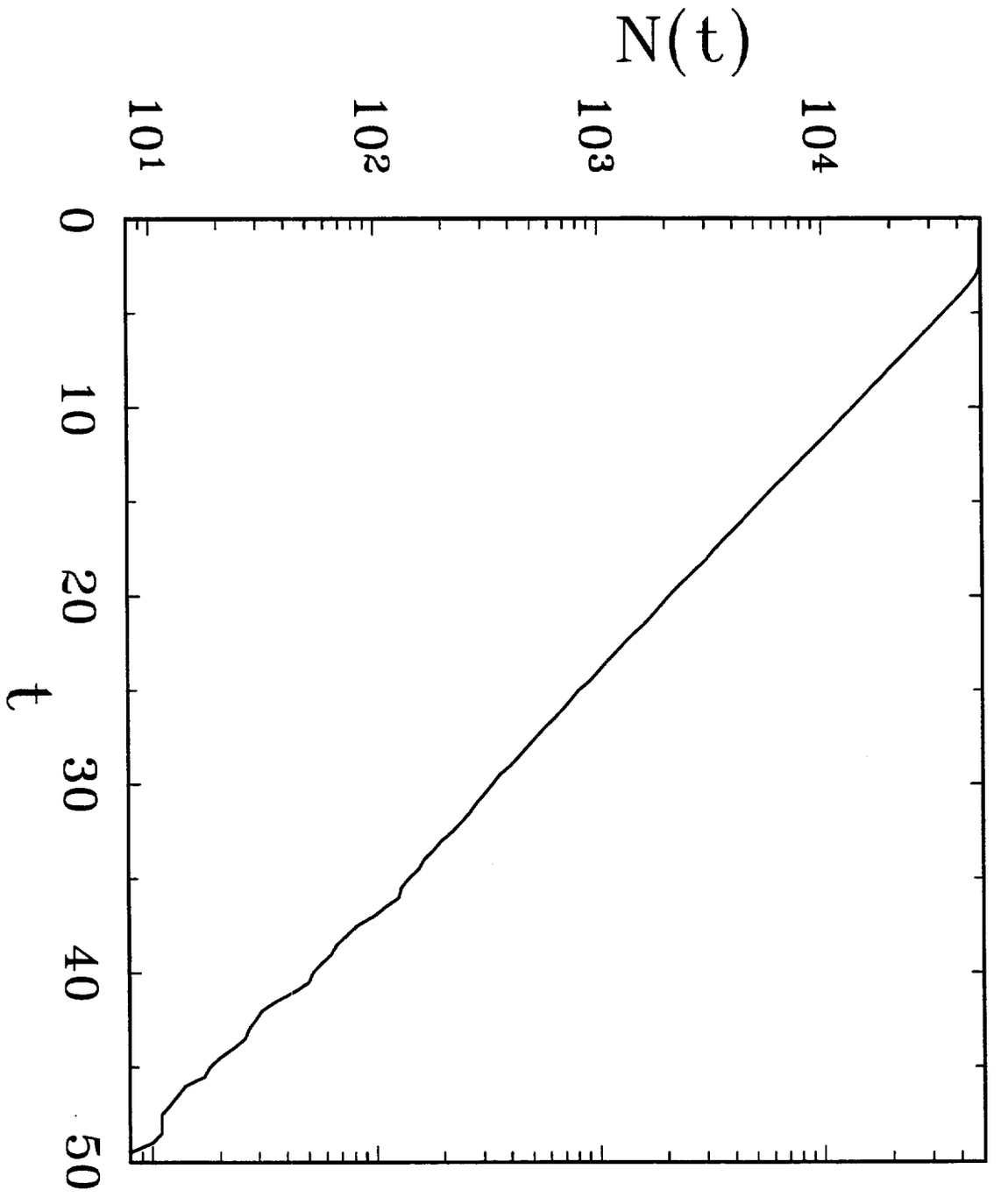

Fig. 9

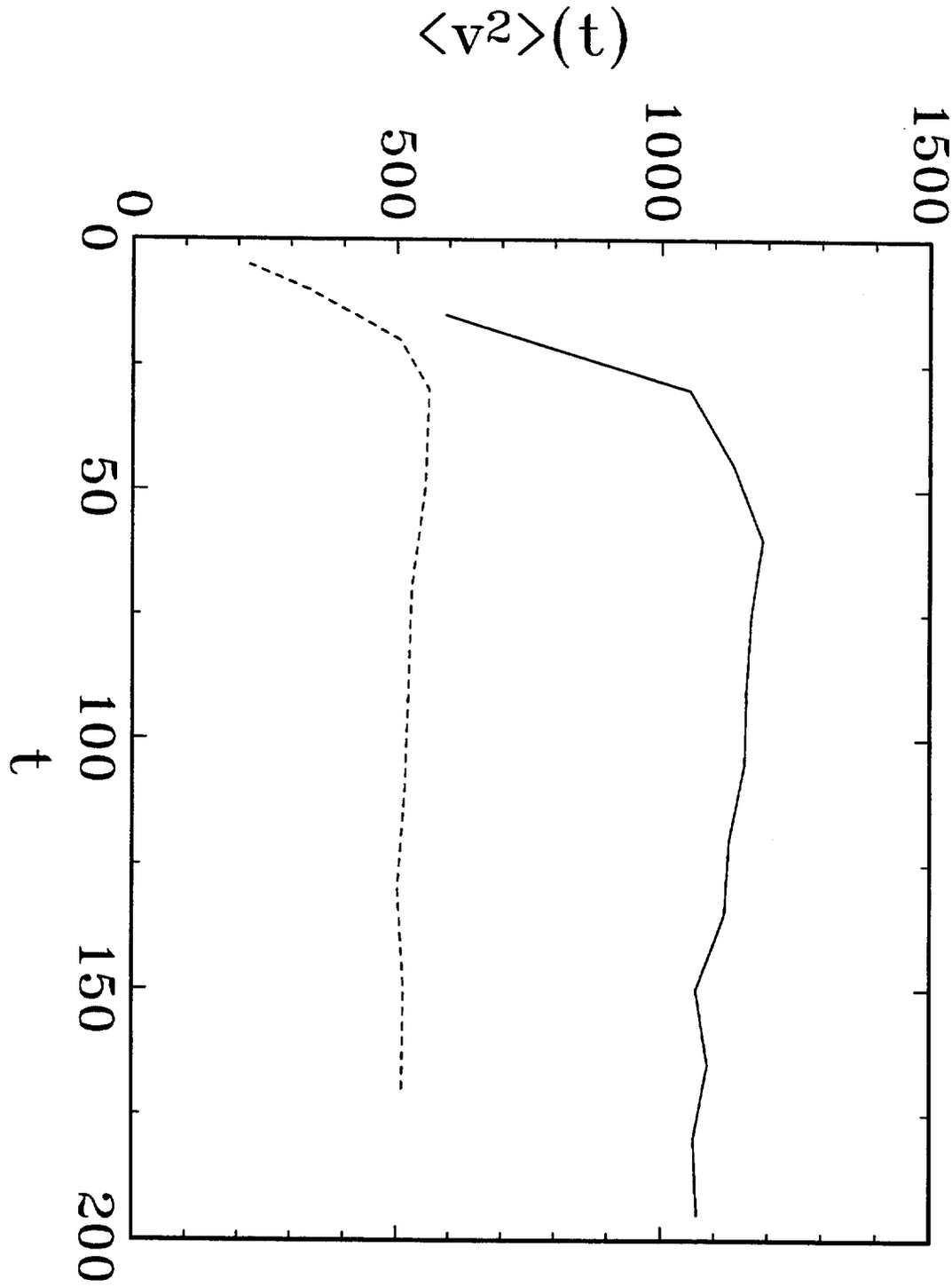

Fig. 10