

# Particle diffusion in the presence of trapping

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The diffusion of particles in the presence of randomly distributed trapping centres is examined. An analytical approach is developed for three simple models of the trap-release processes. It is shown that the particle motion remains diffusive on the average, but the diffusion coefficient can have large fluctuations. The results of the numerical simulations confirm the main qualitative trends found in the analytical study. Although they are very simple, the models can be useful for the examination of the diffusion in tokamak plasma in the presence of quasi-coherent structures which act as trapping centres. © 1997 American Institute of Physics. [S1070-664X(97)03905-0]

## I. INTRODUCTION

Recent theoretical models, based on the ideas of self-organization at criticality of the tokamak plasma, suggest that the stable state of the plasma is necessarily characterized by fluctuations and that a steady continuous state is unstable. This implies that the plasma parameters must be considered as randomly fluctuating quantities rather than continuous ones. First of all, one must note that the fluctuations which are implied by these models are different from those arising from the nonlinear interaction of plasma waves, as considered in the statistical theory of plasma turbulence. The latter are determined by the nonlinear mode coupling which can lead to a stationary state consisting of energy transfer in the spectrum of the excited modes. The former are essentially related to the transient processes of rise and decay of marginally stable waves and represent a source of intermittency.<sup>1</sup>

Both types of fluctuations are competing to establish the shape of the signals which are measured in experiments. In the fully developed turbulence models the saturation occurs when the rate of extraction of the free energy equals the rate of dissipation. In the real case, this situation may not be stationary. Indeed, the current picture of the stationary turbulent states at saturation does not include a proper treatment of the dynamic replacement of the extracted energy. This would require a consistent study of the evolution of the background profiles on the same time scale as the growth of the unstable waves. If the rate of extraction is significantly larger than the rate of local feeding by sources and diffusion, then the plasma will exhibit an intermittent rather than continuous behavior. The excitation of a spectrum of waves will arise in isolated, burst-like events which appear as an additional source of fluctuation of the total signal. On a longer time scale this state would appear however as the stationary stable state of the plasma.

We shall examine in this work a particular type of fluctuation of a variable describing the plasma state. In general terms, we argue that the plasma dynamics can naturally lead to a stationary state in which plasma variables, commonly associated with a statistical description, actually exhibit fluctuations. In this situation it may even be difficult (principally and quantitatively) to find a definite value of these variables.

It is quite common to assume that the scattering of the results arising from a series of measurements of some parameter is due to the imprecision of the experimental method. On a graph this is usually represented as error bars around the statistical average value. While the experimental imprecision is in general unavoidable, it is important to notice that the intrinsic fluctuations of the parameter can be erroneously incorporated into the error bars.

In this work we try to illustrate this idea by studying a simple example of an intrinsically fluctuating plasma variable. Diffusion in the presence of particle trap-release processes provides, besides the modification of the diffusion coefficient, a large fluctuation of the diffusive behavior. As a possible source of trapping we invoke the intermittent rise and decay of quasi-coherent vortices in fully developed ion-temperature gradient driven turbulence.

The ion-temperature gradient driven turbulence have received considerable attention, as it appears as a possible candidate for explaining the ion transport in tokamak.<sup>2</sup> Both the analytical and numerical studies converge to point out the process of dynamical formation of quasi-coherent structures with relatively large spatial extension and finite lifetime. This is consistent with the particular role played by the ion polarization drift which, from the analytical point of view, induces differential properties similar to those which lead to the stable vortex solution of the Hasegawa–Mima equation. As the theory and the numerical simulations show,<sup>3</sup> the stationary state consists of intermittent formation of vortices which move and eventually decay. Then, in terms of a qualitative representation, we can assume that the nonlinear regime of the fully developed turbulence is characterized by quasi-coherent structures which are trying to form but which are not able to arrive at the definite form of the purely nonlinear solution (stable vortex, mono or di-polar). This behavior has been found in the numerical simulation of the nonlinear Schrödinger equation as well.<sup>4</sup> These quasi-coherent structures act as trapping centres and obviously the individual motion of the particles is no longer of the same type as a general Brownian motion. This is well known from the experimental and numerical studies on the transport of impurity contaminants in fluids. The diffusive trajectories of the particles (convected by the fluid motion) are interrupted during finite time sequences when the particle is trapped in the vortices.<sup>5</sup>

We examine analytically and numerically some simple

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models of diffusion with random trapping. Our results show that the motion remains on the average diffusive, but the diffusion coefficient measured in different realizations of the random trapping structure (positions, radii of the vortices and times of residence of the particle in the trap) exhibits large fluctuations. This may arise new questions with regard to the validity of the scaling laws, since they are heavily dependent on the scale invariance of the equations describing the plasma state. For weak external forcing (small additional power injection) and in the regimes where the trap-release processes have a substantial influence on transport, the strong fluctuations of the diffusion may yield a dispersion of the experimental points around the line representing the scaling law.

Our study is mainly qualitative in the sense that the analytical and numerical calculations are limited to simple models. In the following two sections we develop an analytical treatment of the diffusion in the presence of trap-release processes. In the first model the condition of particle number conservation is respected in statistical average and the results show large fluctuations of the diffusion coefficient. The second model conserves the particle number on time scales larger than the fixed duration of residence in a trap. The results show a more reasonable scaling of the fluctuations with time. A more quantitative study is presented in Section IV for the case of ‘‘Lagrangian trapping,’’ i.e., where the statistical properties of the trapping events are specified in terms of the time measured in the frame of the particle. A series of numerical simulations has been carried out in support of the analytical calculations and the results are presented in Section V. The conclusions are discussed in the last section.

## II. RANDOM TRAPPING

In this model, we assume that the particle which arrives at a trapping centre is definitively captured. Since in another point particles are released, we can consider that the centres of trapping have their own motion and that the particles captured in some place, at some time, are released at a later time in another point. To represent analytically this process we introduce a random source in the diffusion equation:

The equation is:

$$\frac{\partial P(x,t)}{\partial t} = D \frac{\partial^2 P(x,t)}{\partial x^2} + \eta(x,t). \quad (1)$$

$P(x,t)$  is the probability density function to find the particle at the point  $x$  at time  $t$  and  $D$  is the diffusion coefficient. To simplify the analytical treatment we restrict to the one-dimensional case but the generalization is obvious. The random source is modelled as:

$$\eta(x,t) = \sum_{\alpha=1}^N V_{\alpha} \delta(x-x_{\alpha}) \delta(t-t_{\alpha}). \quad (2)$$

Here  $\delta$  is the Dirac function. The set  $(x_{\alpha}, t_{\alpha})$  corresponds to the random positions in space and time of the events consisting of trapping or release. We assume that these random variables are distributed according to the Poisson law. The number of particles trapped or released at each event,  $V_{\alpha}$ , is

also a random variable. We assume for simplicity that it can only take two values:  $V_{\alpha} \in \{V_0, -V_0\}$  with equal probability:

$$\mathcal{P}(V_{\alpha}) = \frac{1}{2} [\delta(V_{\alpha} - V_0) + \delta(V_{\alpha} + V_0)]. \quad (3)$$

In the absence of the trap-release processes, the solution of Eq. (1) is the standard diffusion with coefficient  $D$  corresponding to an initial condition which we take as:

$$P(x, t=0) = n_0 \delta(x), \quad (4)$$

where  $n_0$  is the total number of particles. We shall calculate the correlations of the function  $P(x,t)$  by averaging over the distribution of the trapping events and over  $V_{\alpha}$ . In order to perform this calculation systematically we use the generating functional:<sup>6,7</sup>

$$\mathcal{Z} = \int \mathcal{D}[\tilde{P}(x,t)] \mathcal{D}[P(x,t)] \left\langle \exp \left\{ i \int dx dt \right. \right. \\ \left. \left. \times \left[ -\tilde{P} \frac{\partial P}{\partial t} + D \tilde{P} \frac{\partial^2 P}{\partial x^2} + \tilde{P} \eta \right] \right\} \right\rangle_{(x_{\alpha}, t_{\alpha}), V_{\alpha}}. \quad (5)$$

The function  $\tilde{P}(x,t)$  is the conjugate of  $P(x,t)$  (similar to the variables of a Fourier transformation) and  $\mathcal{D}$  is the functional measure. The space and time integrations in the exponent are performed on intervals sufficiently large compared to the spatial region of diffusion and respectively to the time of observation of the system. The averaging is performed separately:

$$\left\langle \exp \left\{ i \int dx dt \tilde{P} \eta \right\} \right\rangle_{(x_{\alpha}, t_{\alpha}), V_{\alpha}} \\ = \left\langle \exp \left\{ i \int dx dt \tilde{P} \sum_{\alpha=1}^N V_{\alpha} \delta(x-x_{\alpha}) \delta(t-t_{\alpha}) \right\} \right\rangle_{(x_{\alpha}, t_{\alpha}), V_{\alpha}} \\ = \left\langle \exp \left\{ i \sum_{\alpha} \tilde{P}(x_{\alpha}, t_{\alpha}) V_{\alpha} \right\} \right\rangle_{(x_{\alpha}, t_{\alpha}), V_{\alpha}}. \quad (6)$$

Denoting this expression by  $E$ , we obtain after averaging over  $V_{\alpha}$  with the probability distribution Eq. (3):

$$E = \left\langle \prod_{\alpha} \exp \{ i \tilde{P}(x_{\alpha}, t_{\alpha}) V_{\alpha} \} \right\rangle_{(x_{\alpha}, t_{\alpha}), V_{\alpha}} \\ = \prod_{\alpha} \langle \cos(V_0 \tilde{P}(x_{\alpha}, t_{\alpha})) \rangle_{(x_{\alpha}, t_{\alpha})} \equiv \prod_{\alpha} \langle \varphi_{\alpha} \rangle. \quad (7)$$

Now, let  $\varphi_{\alpha} \equiv h(x_{\alpha}, t_{\alpha}) + 1$ . The averaging gives (see, for example, Ref. 8):

$$\begin{aligned}
& \left\langle \prod_{\alpha} (h(x_{\alpha}, t_{\alpha}) + 1) \right\rangle \\
&= \exp \left\{ \sum_{\ell=1}^{\infty} \frac{1}{\ell!} \int dx_1 dt_1 \cdots dx_{\ell} dt_{\ell} h(x_1, t_1) \cdots \right. \\
&\quad \left. \times h(x_{\ell}, t_{\ell}) \chi^{(\ell)}(x_1, t_1, \dots, x_{\ell}, t_{\ell}) \right\} \\
&= \exp \left\{ \rho \nu \int dx dt h(x, t) \right\}. \tag{8}
\end{aligned}$$

The higher than first cumulants  $\chi^{(\ell)}$ ,  $\ell \geq 2$ , are zero. The new parameters have the following meaning:  $\nu$  is the inverse of the average time interval between consecutive trapping events and  $\rho$  is the average space density of trapping centres. Returning to Eq. (5) we have:

$$\begin{aligned}
\mathcal{Z} &= \int \mathcal{D}[\tilde{P}(x, t)] \mathcal{D}[P(x, t)] \exp \left\{ i \int dx dt \right. \\
&\quad \left. \times \left[ -\tilde{P} \frac{\partial P}{\partial t} + D \tilde{P} \frac{\partial^2 P}{\partial x^2} - i \rho \nu (\cos(V_0 \tilde{P}) - 1) \right] \right\} \\
&\equiv \int \mathcal{D}[\tilde{P}(x, t)] \mathcal{D}[P(x, t)] \exp \{ i S_{eff} \}.
\end{aligned}$$

In the usual procedure developed for the calculation of  $\mathcal{Z}$  one modifies the action by adding terms of interaction with arbitrary “external currents”  $J_1$  and  $J_2$ :

$$\begin{aligned}
S_{eff}^J[\tilde{P}, P] &= \int dx dt \left[ -\tilde{P} \frac{\partial P}{\partial t} + D \tilde{P} \frac{\partial^2 P}{\partial x^2} \right. \\
&\quad \left. - i \rho \nu (\cos(V_0 \tilde{P}) - 1) + J_1 P + J_2 \tilde{P} \right] \\
&\equiv \int dx dt \mathcal{L}_J. \tag{9}
\end{aligned}$$

After an integration by parts the Lagrangian density is:

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$$\begin{aligned}
\mathcal{L}_J &= \exp \{ i S_{eff}^J[\tilde{P}_0, P_0] \} \\
&= \exp \left\{ \int dx \int dt \left[ J_1(x, t) \frac{n_0}{(4\pi D t)^{1/2}} \exp \left( -\frac{x^2}{4Dt} \right) \Theta(t) - \left( \int_t^{\infty} dt' \int dx' G(x', t'; x, t) J_1(x', t') + A(x, t) \right) \right. \right. \\
&\quad \left. \left. \times i \nu \rho V_0 \sin(V_0 \tilde{P}_0(x, t)) - i \nu \rho \cos(V_0 \tilde{P}_0(x, t)) + i \nu \rho + J_1(x, t) \int_0^t dt' \int dx' i \nu \rho V_0 \sin(V_0 \tilde{P}_0(x, t)) G(x, t; x', t') \right] \right\}, \tag{14}
\end{aligned}$$

where

$$G(x, t; x', t') \equiv \frac{1}{(4\pi D(t-t'))^{1/2}} \exp \left[ -\frac{(x-x')^2}{4D(t-t')} \right]. \tag{15}$$

We have taken  $J_2 = 0$  since in the following calculations we shall only need to perform functional derivatives with respect to  $J_1(x, t)$ .

It is now possible to calculate the average of the function  $P$ , for arbitrary  $(x_0, t_0)$ :

$$\begin{aligned}
\mathcal{L}_J &= -\tilde{P} \frac{\partial P}{\partial t} - D \left( \frac{\partial \tilde{P}}{\partial x} \right) \left( \frac{\partial P}{\partial x} \right) - i \rho \nu (\cos(V_0 \tilde{P}) - 1) \\
&\quad + J_1 P + J_2 \tilde{P}. \tag{10}
\end{aligned}$$

The Euler–Lagrange equations are:

$$\begin{aligned}
\frac{\partial \tilde{P}}{\partial t} + D \frac{\partial^2 \tilde{P}}{\partial x^2} &= -J_1, \\
\frac{\partial P}{\partial t} - D \frac{\partial^2 P}{\partial x^2} &= J_2 + i \nu \rho V_0 \sin(V_0 \tilde{P}). \tag{11}
\end{aligned}$$

Using the standard propagator of the diffusion operator, the solution of the second equation can be written:

$$\begin{aligned}
P_0(x, t) &= \frac{n_0}{(4\pi D t)^{1/2}} \exp \left( -\frac{x^2}{4Dt} \right) \Theta(t) + \int_0^t dt' \int dx' \\
&\quad \times (J_2(x', t') + i \nu \rho V_0 \sin(V_0 \tilde{P}(x', t'))) \\
&\quad \times \frac{1}{(4\pi D(t-t'))^{1/2}} \exp \left[ -\frac{(x-x')^2}{4D(t-t')} \right], \tag{12}
\end{aligned}$$

where  $\Theta$  is the Heaviside function. The solution of the first equation is the adjoint function of the diffusive process:<sup>9</sup>

$$\begin{aligned}
\tilde{P}_0(x, t) &= \int_{t+\epsilon}^{\infty} dt' \int dx' \frac{1}{(4\pi D(t'-t))^{1/2}} \\
&\quad \times \exp \left[ -\frac{(x-x')^2}{4D(t'-t)} \right] J_1(x', t') + A(x, t). \tag{13}
\end{aligned}$$

In Eq. (13)  $A(x, t)$  is everywhere zero at finite times and for  $t = \infty$  this part reproduces the initial condition Eq. (4).

We now consider the lowest order approximation of the functional integral, which simply means that we calculate the action along the solution which minimizes it:

$$\begin{aligned}
\langle P(x_0, t_0) \rangle &= \frac{1}{\mathcal{Z}_J} \frac{\delta \mathcal{Z}_J}{i \delta J_1(x_0, t_0)} \Big|_{J=0} \\
&= \frac{n_0}{(4\pi D t_0)^{1/2}} \exp\left(-\frac{x_0^2}{4D t_0}\right) \\
&\quad + i \nu \rho V_0 \left(-V_0 \frac{d}{dV_0} + 1\right) \\
&\quad \times \int_0^{t_0} dt \int dx G(x_0, t_0; x, t) \sin(V_0 A(x, t)).
\end{aligned} \tag{16}$$

Since for finite times  $A(x, t)$  is identically zero, we obtain as expected the simple diffusive solution as the average of this process [i.e. the first term in the rhs in Eq. (16)].

Now we calculate the correlation of the function  $P(x, t)$  in two points  $(x_0, t_0)$  and  $(x_1, t_1)$ :

$$\langle P(x_0, t_0) P(x_1, t_1) \rangle = \frac{1}{\mathcal{Z}_J} \frac{\delta}{i \delta J_1(x_1, t_1)} \frac{\delta \mathcal{Z}_J}{i \delta J_1(x_0, t_0)} \Big|_{J=0}. \tag{17}$$

In particular, when the points are identical we find:

$$\langle [P(x_0, t_0) - \langle P(x_0, t_0) \rangle]^2 \rangle = \frac{\nu \rho V_0^2}{\sqrt{2\pi D}} t_0^{1/2}. \tag{18}$$

Postponing a detailed discussion of this result we only remark that the root-mean-square deviation of the density increases slowly with time (as  $t^{1/4}$ ) with the same rate for all spatial positions.

In the absence of trapping ( $\eta=0$ ) the diffusive equation (1) represents the stochastic motion of a particle with “white noise” velocity (a classical Brownian motion).  $P(x, t)$  is the probability distribution of the position  $x(t)$  of the particle and the mean-square displacement is:

$$\overline{x^2(t)} \equiv \frac{1}{n_0} \int dx x^2 P(x, t). \tag{19}$$

This quantity can also be used to obtain the diffusion coefficient for a particular realization of the trapping structure. We now calculate its average over the random trapping processes using the statistical properties of  $P(x, t)$  obtained before. This gives:

$$\langle \overline{x^2(t)} \rangle = 2Dt, \tag{20}$$

which means that, when observing a statistical ensemble of realizations of  $x(t)$  one concludes that the motion is diffusive on the average, with the diffusion coefficient  $D$ . However there are significant departures from the *average* diffusive behavior in any observation (due to the stochastic change in the trapping structure). In order to examine the fluctuations around the *average* diffusive behavior, we shall calculate the second cumulant (equivalent to the dispersion) of the stochastic variable  $\overline{x^2(t)}$  averaged over the realizations of the random trapping process. The cumulant is obtained from the two point correlation,  $C$ :

$$\begin{aligned}
n_0^2 C &= \left\langle \int dx_0 x_0^2 P(x_0, t_0) \int dx_1 x_1^2 P(x_1, t_1) \right\rangle \\
&\quad - \left\langle \int dx_0 x_0^2 P(x_0, t_0) \right\rangle \left\langle \int dx_1 x_1^2 P(x_1, t_1) \right\rangle \\
&= \int dx_0 x_0^2 \int dx_1 x_1^2 \langle P(x_0, t_0) P(x_1, t_1) \rangle \\
&\quad - \int dx_0 x_0^2 \langle P(x_0, t_0) \rangle \int dx_1 x_1^2 \langle P(x_1, t_1) \rangle.
\end{aligned} \tag{21}$$

The first term can be calculated using Eq. (17) and the second using Eq. (20):

$$\begin{aligned}
C &= 4\pi \nu \rho V_0^2 D^2 n_0^{-2} \int dx \int dt \Theta(t_0 - t) \Theta(t_1 - t) \\
&\quad \times \left(-V_0 \frac{d}{dV_0} + 1\right) \cos(V_0 A(x, t)) (t_0 - t)(t_1 - t) \\
&\quad \times \left(1 + \frac{2x^2}{4D(t_0 - t)}\right) \left(1 + \frac{2x^2}{4D(t_1 - t)}\right).
\end{aligned} \tag{22}$$

The spatial integration now becomes explicitly related to the volume where trapping occurs, which is intuitively clear. In an imaginary experiment, one releases a number of particles at a certain point. The number of particles arriving at the limit of the volume  $L$  depends on the effect of the random trap-release events in this volume. Taking for simplicity equal times in Eq. (22) we get:

$$\begin{aligned}
&\langle [\overline{x^2(t_0)} - \langle \overline{x^2(t_0)} \rangle]^2 \rangle \\
&= \langle (\overline{x^2(t_0)})^2 \rangle - \langle \overline{x^2(t_0)} \rangle^2 \\
&= \frac{4\pi}{3} \nu \rho V_0^2 D^2 L n_0^{-2} \left( t_0^3 + \frac{1}{2} \frac{t_0^2 L^2}{D} + \frac{3}{20} \frac{t_0 L^4}{D^2} \right).
\end{aligned} \tag{23}$$

The result exhibits a strong dependence on the spatial volume  $L$  where the diffusion takes place. The result that the fluctuations diverges as the volume increases might appear at first sight unexpected. We end this section by a brief discussion of this problem.

In the classical problem of random trapping (and/or multiplication) studied in solid state physics,<sup>10–14</sup> the trapping events are considered either perfect (“trap and die”) or partial (“shallow trappers”). In the first case, the quantity which is calculated is the time-dependent survival probability for an initial density of particles. It is shown that finding the asymptotic decay of the density is equivalent to finding the density of states of a quantum particle in a random potential with singular ( $\delta$ -form) negative peaks located at the trapping centres. The analytical calculation requires consideration of the instanton contribution to the propagator (two-point correlation) which is usually done in the lowest order in the expansion of the action around the extremizing paths, i.e. the instantons.<sup>8</sup> The result is a “stretched exponential” decay of the density of particles, which is rather surprising since it is slower than expected. It has been explained that this behavior is due to the contributions of the large areas with no trapping centres although they are rare in the statistical sense. However, a more detailed calculation<sup>10</sup> which

takes into account the next order in the expansion of the action around the instanton solution has shown that the correction to the lowest order is of the same order of magnitude as the lowest order itself, indicating that there are very large fluctuations. The statistically rare events are not perceived in the averaged result, but they dominate the dynamics through the very large fluctuations. This is precisely what happens in our case: The rare events where most of the centres are trapping (i.e. the value of the random variable  $V_\alpha$  is  $-V_0$  for most of the  $\alpha$ 's) induce large loss of density. Alternatively, the release of particles from most of the centres in one single realization induces a large increase of the density. Since in these cases the centres have identical behaviors, the contributions are proportional to the spatial volume,  $L$ . Naturally, the unbounded increase of the fluctuations with the volume is related, in our treatment, to the absence of a condition of particle number conservation, which is only present in the statistical average of Eq. (1) over the random trapping processes.

We conclude that the preceding results should be considered as qualitative, but nevertheless, that they indicate the presence of large fluctuations in the diffusive behavior of the particle density when the "trap-and-release" processes are included.

### III. TRAPPING WITH FINITE TIME OF RESIDENCE

The expression adopted in the Eq. (2) is the simplest representation of the random trapping as an additive noise in the diffusion equation. One might wonder if the presence of fluctuations of the effective diffusion coefficient is confined to this particular choice. We use in this section a representation of the trapping which, in every realization, ensures the particle number conservation on time scales larger than the time of residence in a trap. As a result, the time dependence of the statistical quantities is reversed (the fluctuations quench asymptotically). However the main issue is the persistence, in this more realistic model, of a substantial level of fluctuations with a slow (algebraic) time decay.

We consider instead of Eq. (2) a random series of events consisting of trapping followed by release:

$$\eta(x, t) = \sum_{\alpha} V_{\alpha}(t, t_{\alpha}) \delta(x - x_{\alpha}), \quad (24)$$

where

$$V_{\alpha}(t, t_{\alpha}) = -V_0 \delta\left(t - t_{\alpha} + \frac{\zeta}{2}\right) + V_0 \delta\left(t - t_{\alpha} - \frac{\zeta}{2}\right). \quad (25)$$

This means that the particle is trapped at the moment  $t_{\alpha} - \zeta/2$  and released in the same point  $x_{\alpha}$  at the moment  $t_{\alpha} + \zeta/2$ . Using the same analytical approach as before, we perform the averaging over the new form of the noise:

$$\begin{aligned} & \left\langle \exp\left(i \int dx dt \tilde{P} \eta\right) \right\rangle_{(x_{\alpha}, t_{\alpha})} \\ &= \exp\left\{ \nu \rho \int dx dt \right. \\ & \quad \times \left[ \exp\left(i V_0 \tilde{P}\left(x, t + \frac{\zeta}{2}\right) - i V_0 \tilde{P}\left(x, t - \frac{\zeta}{2}\right)\right) - 1 \right] \Big\}. \end{aligned} \quad (26)$$

The Lagrangian becomes:

$$\begin{aligned} \mathcal{L}_J = & -\tilde{P} \frac{\partial P}{\partial t} - D \left( \frac{\partial \tilde{P}}{\partial x} \right) \left( \frac{\partial P}{\partial x} \right) - i \nu \rho \left[ \exp\left(i V_0 \right. \right. \\ & \times \tilde{P}\left(x, t + \frac{\zeta}{2}\right) - i V_0 \tilde{P}\left(x, t - \frac{\zeta}{2}\right) \Big) - 1 \Big] + J_1 P + J_2 \tilde{P}. \end{aligned} \quad (27)$$

The shifted arguments of the functions appearing in the Lagrangian lead to analytical difficulties. We can simplify the problem by restricting our attention to those cases where the time of residence in a trap  $\zeta$  is small compared to the "time of observation." This allows to expand the functions around the centre of the interval of trapping:

$$\begin{aligned} \mathcal{L}_J = & -\tilde{P} \frac{\partial P}{\partial t} - D \left( \frac{\partial \tilde{P}}{\partial x} \right) \left( \frac{\partial P}{\partial x} \right) - i \nu \rho \left[ \exp\left(i V_0 \zeta \frac{\partial \tilde{P}}{\partial t}\right) - 1 \right] \\ & + J_1 P + J_2 \tilde{P}. \end{aligned} \quad (28)$$

The Euler-Lagrange equations are:

$$\begin{aligned} \frac{\partial \tilde{P}}{\partial t} + D \frac{\partial^2 \tilde{P}}{\partial x^2} &= -J_1, \\ \frac{\partial P}{\partial t} - D \frac{\partial^2 P}{\partial x^2} &= J_2 - i \nu \rho V_0^2 \zeta^2 \frac{\partial^2 \tilde{P}}{\partial t^2} \exp\left(i V_0 \zeta \frac{\partial \tilde{P}}{\partial t}\right). \end{aligned} \quad (29)$$

In order to solve these equations, we perform an approximation which is valid for small time of residence in a trap, i.e. expand in Eq. (28) the exponential and retain the first order term. The details of the calculations are given in the Appendix.

As before, we are interested in the average value of the particle density  $P(x, t)$  in an arbitrary point. We find:

$$\langle P(x, t) \rangle = \frac{1}{\mathcal{Z}_J} \frac{\delta \mathcal{Z}_J}{i \delta J_1(x, t)} \Big|_{J=0} = \frac{n_0}{(4 \pi D t)^{1/2}} \exp\left[-\frac{x^2}{4 D t}\right], \quad (30)$$

which shows that the motion of the particle is diffusive and that, in our approximation, the coefficient is  $D$ . To find the fluctuations around the diffusive motion we calculate:

$$\begin{aligned} \langle (P(x, t))^2 \rangle &= \frac{1}{\mathcal{Z}_J} \frac{\delta}{i \delta J_1(x, t)} \frac{\delta}{i \delta J_1(x, t)} \mathcal{Z}_J \Big|_{J=0} \\ &= \left( \frac{n_0}{(4 \pi D t)^{1/2}} \exp\left[-\frac{x^2}{4 D t}\right] \right)^2 \\ & \quad + \text{const} \times \nu \rho V_0^2 \zeta^2 D^{-1/2} t^{-3/2}, \end{aligned} \quad (31)$$

where the first term in the right hand side is  $\langle P(x,t) \rangle^2$ . The numerical constant results from integrations of degenerate hypergeometric functions.

The dispersion of the random profiles  $P(x,t)$  around the average one, while remaining substantial in certain range of parameters, exhibits a slow (algebraic) decay. This is opposed to the time growth obtained previously, Eq. (18), and is related to the property of the noise Eq. (24) of conserving the number of particles. The global impact of the random trap-release processes on the diffusion relies on statistically rare events consisting in massive trapping or massive release of particles, as explained at the end of the previous section. Since in the model of noise these events follow each other, the effect is bounded to an average value. Quantitatively, the weight of these events decays with the increase of the area of diffusion [i.e.,  $(Dt)^{1/2}$ ] and as the ratio of the total time of residence and the time  $t$  of observation.

#### IV. LAGRANGIAN MODEL OF TRAPPING

Let us review the case treated in the preceding sections, but now, from the point of view of the particle motion. The particle performs diffusive motion in the presence of traps distributed randomly in the volume. We assumed that, once the particle arrives at a trap, it is absorbed and remains there for a certain time before being released to continue its diffusive motion. We considered that the duration of residence in a trap is a constant,  $\zeta$ . To completely specify the problem, we need the diffusion coefficient of the motion between the traps and the law of distribution of the positions of the trapping centres. We shall refer to the problem in this setting as the ‘‘Eulerian problem.’’ Alternatively, we adopt an approach in which the moments  $\tau_i$  (when the particle encounters a trap) obey a distribution law expressed as a function of the time measured in the frame of the particle (the ‘‘Lagrangian problem’’). In this case the spatial positions of the trapping centres are no more important.<sup>15</sup> Assuming that the distribution of  $\tau_i$ 's is the Poisson's law, we shall calculate the mean-square displacement (MSD) of a particle which performs diffusive motion interrupted at random by trapping events of fixed duration  $\Delta$ . The Langevin equation is

$$\dot{x}(t) = \eta_{tr}(t) = \begin{cases} \eta(t) & \text{for } t \notin \cup_i (\tau_i, \tau_i + \Delta), \\ 0 & \text{for } t \in \cup_i (\tau_i, \tau_i + \Delta), \end{cases} \quad (32)$$

and  $\langle \eta(t) \eta(t') \rangle = 2D \delta(t - t')$ . The following notation is useful:

$$\dot{x}(t) = \eta(t)H(t),$$

$$H(t) \equiv 1 - \sum_{i=1}^N \Theta(t - \tau_i) \Theta(\tau_i + \Delta - t). \quad (33)$$

The Langevin-type equation is solved using the functional formalism. We introduce the generating functional which now takes the form:

$$\mathcal{Z} = \int \mathcal{D}[x(t)] \mathcal{D}[k(t)] \exp \left\{ i \int_0^T dt [-\dot{x}(t)k(t)] \right\} \\ \times \left\langle \exp \left\{ i \int_0^T dt k(t) \eta(t) H(t) \right\} \right\rangle, \quad (34)$$

where the average is taken over the noise  $\eta(t)$  and the distribution of points  $\tau_i$ . Since  $\eta$  is white noise we can write:

$$\left\langle \exp \left\{ i \int_0^T dt k(t) \eta(t) H(t) \right\} \right\rangle \\ = \left\langle \exp \left\{ -D \int_0^T dt k(t)^2 + \sum_{i=1}^N D k(\tau_i)^2 \right\} \right\rangle_{\tau_i} \\ = \exp \left\{ \int_0^T dt [-Dk(t)^2 + \nu(\exp(D\Delta k(t)^2) - 1)] \right\}, \quad (35)$$

with  $\nu$  the mean frequency of the trapping events. The averaging over the distribution of the random moments  $\tau_i$  is carried out as in the previous sections. In Eq. (35) we have assumed that  $\Delta \ll \nu^{(-1)}$  i.e., the time of residence is much smaller than the period between the trapping events. This allows us to use the simplest (‘‘rectangle’’) approximation of the integral of  $k(t)$  over the time of residence. Again, we insert the term of interaction of the ‘‘field’’  $x(t)$  with an arbitrary external current  $J(t)$ . The generating functional becomes:

$$\mathcal{Z}_J = \int \mathcal{D}[x(t)] \mathcal{D}[k(t)] \exp \left\{ i \int dt [-\dot{x} + Jx + iDk^2 + i\nu(1 - \exp(\Delta Dk^2))] \right\}. \quad (36)$$

We remark that the integration over the functional variable  $x(t)$  can be carried out after an integration by parts of the first term in the exponent. This leads to a functional- $\delta$ :  $\delta[k(t) - \int_t^T dt' J(t')]$ . Now the integration over  $k(t)$  can be performed with the result:

$$\mathcal{Z}_J = \exp \left\{ - \int_0^T dt \left[ D \left( \int_t^T dt' J(t') \right)^2 + \nu \left( 1 - \exp \left( \Delta D \left( \int_t^T dt' J(t') \right)^2 \right) \right) \right] \right\}. \quad (37)$$

The normalization constant is unity:

$$\mathcal{Z}_{J=0} = 1. \quad (38)$$

The statistical properties of  $x(t)$  can be obtained through functional differentiations:

$$\langle x(t) \rangle = \frac{1}{\mathcal{Z}_J} \frac{\delta \mathcal{Z}_J}{\delta J(t)} \Big|_{J=0} = 0 \quad (39)$$

and

$$\langle x(t)^2 \rangle = \frac{1}{\mathcal{Z}_J} \frac{\delta}{\delta J(t)} \frac{\delta}{\delta J(t)} \mathcal{Z}_J \Big|_{J=0} = 2D(1 - \nu\Delta)t. \quad (40)$$

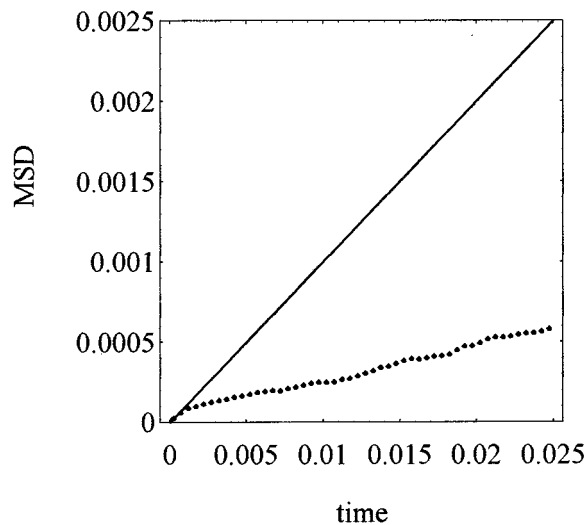


FIG. 1. Time dependence of the mean-square displacement (MSD) averaged over 500 realizations of the random walk, for the case without trapping (continuous line) and for a large "trapping strength" (dotted line).

The decrease of the diffusion coefficient can be important for large residence time and for large number of trapping centres. However, the regime of very dense trapping must be examined without the approximations which are used in the above treatment.

## V. NUMERICAL SIMULATIONS

The numerical simulations permit us to go beyond the restrictive assumptions of the analytical treatments presented above. The diffusion takes place in plane and the trapping centres are represented by circles. For a given average density of centres, their positions are randomly spread in the plane in such a way that the density fluctuations have Poisson distribution. The radii of the circles and the duration of residence in every trap are random with specified (uniform or Gaussian) distribution. A statistical ensemble of realizations of the random trapping structure is then characterized by the three parameters associated to the functions of distribution of the density of centres, the radii and the times of residence. Quantities depending directly on these parameters will be denoted shortly as "trapping strength."

In the first series of runs (A) 500 particles perform  $10^5$  steps of Gaussian diffusion in plane with a fixed distribution of trapping centres obeying the Poisson law. The radii of the circles where trapping occurs and the durations of trapping are chosen at random and then are multiplied with constant factors in several runs. The mean-square displacement depends linearly on time (i.e. the motion is diffusive) even for large trapping effect. In Fig. 1 the diffusion coefficient in the absence of trapping is  $D = 0.1 \text{ m}^2/\text{s}$  and the largest trapping effect corresponds to the largest multiplicative factors. For increasing factors the diffusion coefficient obtained by linear regression exhibits the expected decrease but also shows fluctuations (Fig. 2).

The second case (B) corresponds with several realizations of the trapping structure: The positions are distributed in each realization such that the density of the trapping cen-

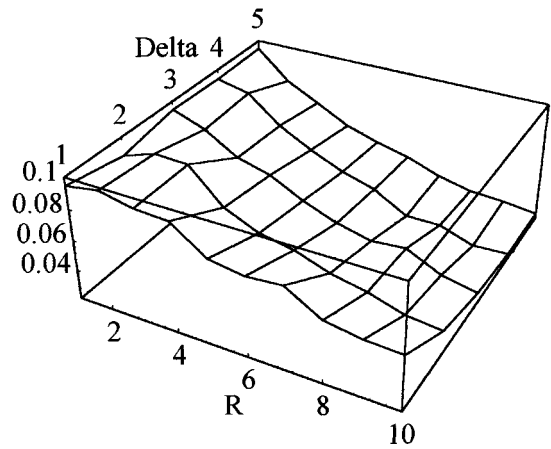


FIG. 2. Case A: Fixed trapping structure and scaling of the areas and of the times of residence. Dependence of the diffusion coefficient with respect to the scaling factors applied on the radii and respectively on the times of residence in the trapping areas.  $R$  is the radius normalized to the initial value and  $\Delta$  is the normalized time of residence.

tres fluctuates obeying the Poisson law. The radii and the times of residence are chosen at random with Gaussian distribution around fixed values. Figure 3 shows the diffusion coefficients obtained in 20 realizations of the random trapping structure. One notes the large fluctuations around the average values.

As explained before, it may be expected that in real experiments the intrinsic fluctuations can be erroneously attributed to the imprecision of the experimental method. In order to examine the order of magnitude of the apparent error bars due to the intrinsic fluctuations we have performed a series of runs (C) which combines the previous ones (A and B).

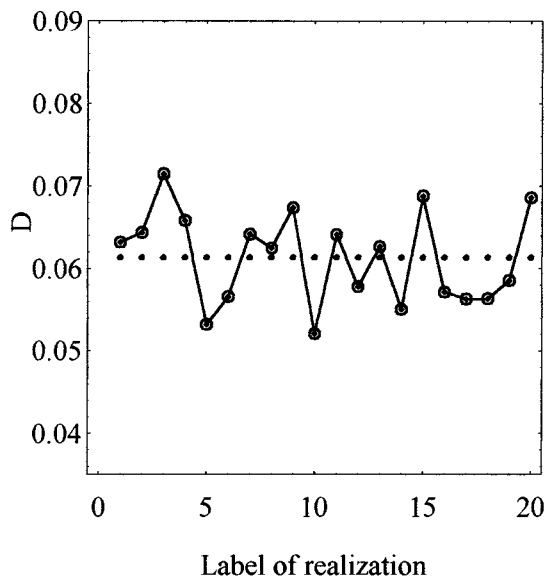


FIG. 3. Case B: Twenty realizations of the random distribution of the trapping centres on the plane. The diffusion coefficients  $D$  obtained in the realizations are shown. The dotted line represents the diffusion coefficient averaged over these realizations, and it is plotted in order to exhibit the differences with the actual values.

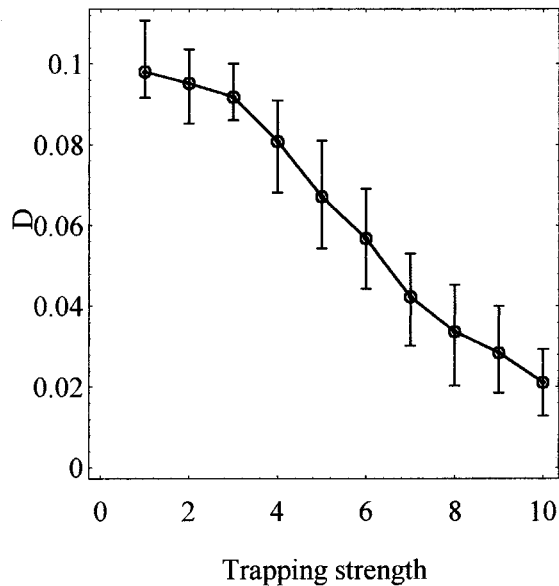


FIG. 4. Case C: Both the trapping effectiveness (through the scaling factor of the radii and the times of residence) and the random realizations are sampled. The average diffusion coefficient is plotted as function of the scaling factor (i.e. the “trapping strength”). The fluctuations of the diffusion coefficient in the various realizations of the random trapping structure are shown as error bars.

Namely, we consider again a structure of random trapping centres, and scale the radii and the times of residence by a constant factor in ten steps, thus obtaining an increasing “trapping strength.” For each step, we allowed 20 realizations of the random distribution of centres (obeying the Poisson law). The diffusion coefficients are calculated in each case. The average values of the diffusion coefficients over the ensemble of realizations are plotted versus the current step in the scaling procedure (Fig. 4). The minimum and maximum values in each realization are also plotted as error bars.

Finally a series of runs (D) was performed in order to check the validity of the analytical result obtained in the “Lagrangian trapping” problem. In order to examine the parametric dependence, we vary the average duration of the diffusive motion between two successive events of trapping ( $1/\nu$ ) by changing the number of the trapping centres. In addition we change the average duration of residence in a trap,  $\Delta$ , and obtain several values of the parameter  $\nu\Delta$ . In Fig. 4 we plot the diffusion coefficients obtained numerically together with the theoretical result Eq. (40). The linear dependence is reproduced reasonably well, but the whole set of numerical results is shifted compared with the analytical result. This difference can be attributed to the assumption adopted in Section IV that the trapping events are distributed along the “time of the particle” according to the Poisson law, while the distribution which has been obtained in the numerical simulation is different.

## VI. CONCLUSIONS

Using simple models we have investigated analytically and numerically the effect of the random trapping on the

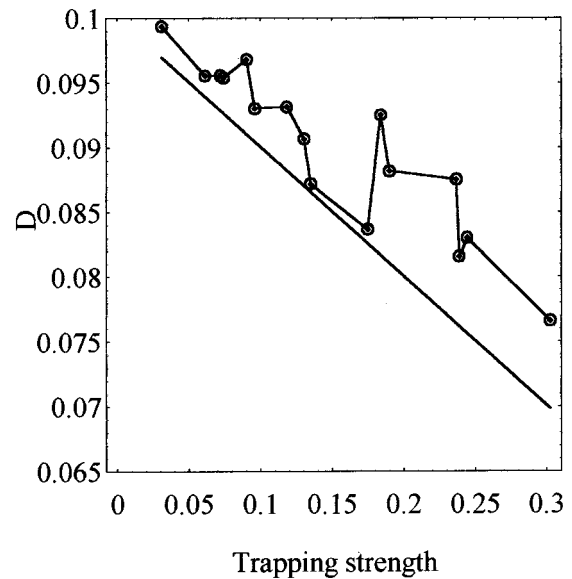


FIG. 5. Case D: Comparison between the numerical result (circles) and the theoretical formula Eq. (40) (the straight line). The “trapping strength” here is  $\nu\Delta$ .

diffusion coefficient. We studied the finite time trapping since it may be relevant for the diffusion of particles in turbulent plasma where vortex structures can form and live for finite time. Previous experimental and numerical studies have shown that the vortices trap particles, and convect them along their own motion. The particles can be released from a vortex either because of the diffusion from inside the vortex core to the external region or because of the destruction of the vortex. It is natural to assume that in fully developed turbulence, the vortical structures are not stable. The effective diffusion coefficient obtained in the presence of trapping is smaller than the value given by the basic diffusive mechanism. The main point, emphasized by our calculations, is that this diffusion coefficient is also a fluctuating quantity.

The absolute values of the averaged diffusion coefficient and the fluctuations are clearly dependent (as shown by the models examined in this work) on the rate of condensation of vortices and on their duration of life. Several preliminary problems must be examined if we want to obtain quantitative results applicable to experiments on the plasma transport in tokamak. The first concerns the possibility of a clear separation between the basic diffusion mechanism and the trapping events. The common situation is that the particle is transported by the random scattering in the potential fluctuations of an electrostatic instability. The characteristic wavelength in the spectrum and the time-scale of the fluctuations must be smaller than the dimension of the vortex and respectively than its lifetime. If these conditions are fulfilled one may consider to use the amplitude of the fluctuations of the diffusion coefficient to estimate the “trapping strength.” In the simple cases we have treated this appears as  $\nu\rho V_0^2$  [in Eq. (23)] and  $\nu\rho V_0^2 \zeta^2$  [in Eq. (31)]. If the trapping structures cannot be distinguished from the potential fluctuations the particle transport enter the so-called “percolation regime,”

where the diffusion coefficient depends on the amplitude of the field weaker than linear.<sup>16,17</sup>

An interesting possibility is suggested by Eq. (40) which shows the decrease of the diffusion coefficient in the presence of trapping. If the turbulent fluctuations of a plasma instability evolves into a regime where quasi-coherent structures (vortices) can form, then the particle transport may decrease. The present models of plasma transport should be modified to take into account the trapping.

The result that the effective diffusion coefficient is fluctuating can be extrapolated and suggests that most plasma variables should be regarded as intrinsically fluctuating quantities. In the experimental studies these fluctuations contribute to the scattering of the raw data in a similar way as the imprecision of the measurement. As a result they are usually contained in the error bars while in fact they correspond to the statistical properties of a particular underlying process.

In fusion plasma this idea may be associated to the intrinsic fluctuations of the plasma variables near the marginally stable state, as suggested by the recent theories of self-organized plasmas.

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## APPENDIX: THE GENERATING FUNCTIONAL FOR TRAPPING WITH FINITE TIME OF RESIDENCE

We point out the behavior in a limiting case of the generating functional based on the Lagrangian given in Eq. (28). As we have seen in Section II, the expression of the generating functional  $\mathcal{Z}_J = \exp[i\int dx dt \mathcal{L}_J]$  differs from the purely diffusive case by the effect of the additional term resulting from the averaging over the random trapping events. If we assume, *a priori*, that the effect of trapping represents a small correction to the diffusive behavior, we can adopt an approximation of the additional term expanding the exponential in the Lagrangian. This yields to the following expression of  $\mathcal{Z}_J$ :

$$\begin{aligned} \exp\left\{\nu\rho\int dx dt\left[\exp\left(iV_0\xi\frac{\partial\tilde{P}}{\partial t}\right)-1\right]\right\} \\ \approx \exp\left\{\nu\rho\int dx dt(iV_0\xi)\frac{\partial\tilde{P}}{\partial t}\right\} \\ = \exp\left\{i\nu\rho V_0\xi\int dx[\tilde{P}(x,t=\infty)-\tilde{P}(x,t=0)]\right\} \\ = \exp\{i\nu\rho V_0\xi L/n_0\}, \end{aligned} \quad (\text{A1})$$

where as before  $L$  denotes the one-dimensional spatial volume. In the last line of Eq. (A1), we used the values at the limits of the function  $\tilde{P}$ : At  $t=0$  it is zero, while at the limit  $t=\infty$  it reproduces the initial density  $P(x,t=0)$  (we also take into account the normalization which renders the action  $\mathcal{S}$  nondimensional). We remark that the part related to the trapping process gives in this limit a simple complex number i.e., a phase factor for  $\mathcal{Z}_J$ . It shows that for particular combinations of the physical parameters  $\nu\rho V_0\xi L/n_0 = (2k+1)\pi/2$  with  $k$  integer the real part of the generating functional  $\mathcal{Z}_J$  vanishes. The physical meaning is obvious: If the number of particles which on the average is trapped at any moment of time equals the total number of particles, then, there are no particles left to diffuse. Naturally we are far from this situation in usual cases and in particular our treatment is only valid in the limit  $\nu\rho V_0\xi L/n_0 \ll 1$ .

We shall perform our analysis starting from the approximation of the Lagrangian which consists in retaining the second order in the expansion of the exponential. This gives:

$$\begin{aligned} \mathcal{L}_J \approx -\tilde{P}\frac{\partial P}{\partial t} - D\left(\frac{\partial\tilde{P}}{\partial x}\right)\left(\frac{\partial P}{\partial x}\right) \\ + \frac{1}{2}i\nu\rho V_0^2\xi^2\left(\frac{\partial\tilde{P}}{\partial t}\right)^2 + J_1P + J_2\tilde{P}, \end{aligned} \quad (\text{A2})$$

and the Euler-Lagrange equations are:

$$\begin{aligned} \frac{\partial\tilde{P}}{\partial t} + D\frac{\partial^2\tilde{P}}{\partial x^2} &= -J_1, \\ \frac{\partial P}{\partial t} - D\frac{\partial^2 P}{\partial x^2} &= J_2 - i\nu\rho V_0^2\xi^2\frac{\partial^2\tilde{P}}{\partial t^2}. \end{aligned} \quad (\text{A3})$$

Using the same notations as in Section II we write the solutions:

$$\begin{aligned} P_0(x,t) &= \frac{n_0}{(4\pi Dt)^{1/2}} \exp\left[-\frac{x^2}{4Dt}\right] \\ &+ \int dt' \int dx' \frac{\Theta(t-t')}{[4\pi D(t-t')]^{1/2}} \\ &\times \exp\left[-\frac{(x-x')^2}{4D(t-t')}\right] \\ &\times \left(J_2(x',t') - i\nu\rho V_0^2\xi^2\frac{\partial^2\tilde{P}(x',t')}{\partial t'^2}\right), \end{aligned} \quad (\text{A4})$$

$$\begin{aligned} \tilde{P}_0(x,t) &= A(x,t) + \int dt' \int dx' \frac{\Theta(t'-t)}{[4\pi D(t'-t)]^{1/2}} \\ &\times \exp\left[-\frac{(x'-x)^2}{4D(t'-t)}\right] J_1(x',t'). \end{aligned} \quad (\text{A5})$$

To examine the leading effect of trapping on the diffusion we can limit our calculations to the lowest order in the expansion of the action functional  $S$  around the extremizing “paths” given in the Eqs. (A4) and (A5). This simply means to replace the solutions obtained above in the expression of the generating functional:

$$\begin{aligned}
\mathcal{L}_J = & \exp \left[ i \int dt \int dx \frac{n_0}{(4\pi Dt)^{1/2}} \exp \left[ -\frac{x^2}{4Dt} \right] J_1(x, t) + i \nu \rho V_0^2 \zeta^2 \int dt \int dx \left[ A(x, t) \frac{\partial^2 A(x, t)}{\partial t^2} + \frac{1}{2} \left( \frac{\partial A(x, t)}{\partial t} \right)^2 \right] \right. \\
& - \nu \rho V_0^2 \zeta^2 \int dt \int dx \int dt' \int dx' \left[ A(x, t) \frac{\partial^2}{\partial t^2} \left( \frac{\Theta(t' - t)}{[4\pi D(t' - t)]^{1/2}} \exp \left[ -\frac{(x' - x)^2}{4D(t' - t)} \right] J_1(x', t') \right) \right. \\
& + \left. \frac{\partial A(x, t)}{\partial t} \frac{\partial}{\partial t} \left( \frac{\Theta(t' - t)}{[4\pi D(t' - t)]^{1/2}} \exp \left[ -\frac{(x' - x)^2}{4D(t' - t)} \right] J_1(x', t') \right) \right] - \frac{1}{2} \nu \rho V_0^2 \zeta^2 \int_0^T dt \int dx \int_0^T dt' \int dx' \int_0^T dt'' \int dx'' \\
& \times \left. \frac{\partial}{\partial t} \left( \frac{\Theta(t' - t)}{[4\pi D(t' - t)]^{1/2}} \exp \left[ -\frac{(x' - x)^2}{4D(t' - t)} \right] J_1(x', t') \right) \times \frac{\partial}{\partial t} \left( \frac{\Theta(t'' - t)}{[4\pi D(t'' - t)]^{1/2}} \exp \left[ -\frac{(x'' - x)^2}{4D(t'' - t)} \right] J_1(x'', t'') \right) \right]. \quad (\text{A6})
\end{aligned}$$

The role of the terms composing the expression in the exponential becomes more transparent if we have in mind that the low order correlations are obtained by taking functional derivatives with respect to the current  $J_1(x, t)$ . We first remark that the term containing products of two factors  $A(x, t)$  has no contribution to the correlations since it does not depend on the current  $J_1(x, t)$ . In addition, an integration by part shows that this term can at most contribute with a constant in the exponential which has no practical consequence due to the normalization.

To emphasize more clearly the terms containing a single factor  $J_1(x, t)$  we perform an integration by parts on the variable  $t$  in the third integral in the exponent:

$$A(x, t) \frac{\partial^2}{\partial t^2} \cdot + \frac{\partial A(x, t)}{\partial t} \frac{\partial}{\partial t} \cdot \rightarrow \frac{\partial}{\partial t} \left( A(x, t) \frac{\partial}{\partial t} \cdot \right).$$

After carrying out the integration on the variable  $t$  we employ the boundary conditions for  $A(x, t)$  i.e.:  $A(x, t=0)=0$  and  $A(x, t=\infty)=(L/n_0)\delta(x)$ . We conclude that within the approximations which lead to the expression of the Lagrangian Eq. (A2) we cannot find a linear term in the current  $J_1$  in the exponent, other than the unperturbed diffusive term [the first line in Eq. (A6)]. This is an important remark, indicating that in order to find corrections to the diffusion coefficient

we must give a more accurate expression of the Lagrangian. Or, alternatively, we must try a different approach, as will be done in the Section IV.

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