Averaged residence times of stochastic motions in bounded domains

O. Bénichou(∗), M. Coppey1, M. Moreau1, P. H. Suet1 and R. Voituriez2

1 Laboratoire de Physique Théorique des Liquides (CNRS UMR 7600)
Université Pierre et Marie Curie - 4 place Jussieu, case courrier 121,
75255 Paris Cedex 05, France
2 Institut Curie - 26 rue d’Ulm, 75248 Paris Cedex 05, France

received 17 January 2005; accepted in final form 10 February 2005
published online 9 March 2005

PACS. 05.40.Fb – Random walks and Levy flights.
PACS. 05.40.-a – Fluctuation phenomena, random processes, noise, and Brownian motion.
PACS. 02.50.-r – Probability theory, stochastic processes, and statistics.

Abstract. – Two years ago, Blanco and Fournier [1] reported an important result concerning the mean first exit time of a domain of a particle undergoing a randomly reoriented ballistic motion which starts from the boundary. They showed that it is simply related to the ratio of the volume’s domain over its surface. This work was extended by Mazzolo [5], who studied the case of trajectories which start inside the volume. In this letter, we propose an alternative formulation of the problem which allows us to calculate not only the mean exit time, but also the mean residence time inside a sub-domain. The cases of any combinations of reflecting and absorbing boundary conditions are considered. Lastly, we generalize our results for a wide class of stochastic motions.

Introduction. – Recently, motivated by the study of diffusive trajectories performed by animals in various conditions, Blanco and Fournier [1] reported an important result concerning the mean first exit time of Pearson random walks [2] in a bounded domain. Beyond the applications for animal trajectories, numerous physical systems are concerned, such as the neutron scattering processes [3,4]. Pearson random walks can be defined by the trajectory of a particle which is submitted at stochastic times to random reorientations of the direction of its constant velocity \(v\). The stochastic times are exponentially distributed with mean value \(1/\lambda\). For this category of random walks, Blanco and Fournier showed that the mean first exit time \(\langle t \rangle\) of a random walk starting from the boundary of a finite domain is independent of the frequency \(\lambda\) and is simply related to the ratio of the domain’s volume \(V\) over the surface \(S\) of the domain’s boundary, namely in three dimension:

\[
\langle t \rangle = \frac{4V}{vS}.
\]

The fact that this result does not depend on the frequency \(\lambda\) but only on the geometry of the system seems counter-intuitive, although Blanco and Fournier propose some heuristic explanation for it. Very recently, following the demonstration of Blanco and Fournier, Mazzolo [5]

(∗) E-mail: benichou@lptl.jussieu.fr
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extended their results and gave a relation between the \( n \)-th moment of the first exit time of a particle starting inside the domain, and the \((n+1)\)-th moment of the first exit time of a particle starting from the boundary.

In this paper, we present an alternative approach, which allows us to extend these results in three directions. First, we consider the case of any combination of absorbing and reflecting boundary conditions, which is useful in many applied stochastic processes. Second, we study not only first exit time properties, but also residence time within sub-domain properties (prior to the first exit of the domain), which is a more general quantity. Last, we show that these results can be generalized for a wide class of stochastic motions.

**First exit time.** Before considering the case of a general motion, we restrict our discussion to the previously examined Pearson walks, which correspond to a succession of deterministic ballistic movements in the bounded domain \( V \) delimited by an absorbing boundary \( \Sigma \), interrupted by instantaneous and isotropic redistributions of the velocity \( \bar{v} \). Let \( p(\bar{r}, \bar{v}, t|\bar{r}, \bar{v}) \) be the conditional density probability at time \( t \) that the particle is at position \( \bar{r} \) with a velocity \( \bar{v} \), given that it starts initially at position \( \bar{r} \) with a velocity \( \bar{v} \). This quantity satisfies the well-known backward Chapman-Kolmogorov differential equation [6]

\[
\partial_t p(\bar{r}, \bar{v}, t|\bar{r}, \bar{v}) = \bar{v} \cdot \nabla_{\bar{r}} p(\bar{r}, \bar{v}, t|\bar{r}, \bar{v}) + \frac{\lambda}{\sigma_d} \int d\bar{v}' [p(\bar{r}, \bar{v}', t|\bar{r}, \bar{v}) - p(\bar{r}, \bar{v}', t|\bar{r}, \bar{v})],
\]

where \( \sigma_d = \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \) stands for the solid angle in \( d \)-dimension and the integral \( \int d\bar{v} \) is taken over unit vectors in the direction of the velocity. This equation can be easily converted into an equation for the moments of the first exit time \( T(\bar{r}, \bar{v}) \) starting from \( \bar{r} \) with the initial velocity \( \bar{v} \) [7]:

\[
\bar{v} \cdot \nabla_{\bar{r}} t_n(\bar{r}, \bar{v}) + \frac{\lambda}{\sigma_d} \int d\bar{v}' (t_n(\bar{r}, \bar{v}') - t_n(\bar{r}, \bar{v})) = -nt_{n-1}(\bar{r}, \bar{v}),
\]

where \( t_n(\bar{r}, \bar{v}) \) is the \( n \)-th moment of the first exit time, which verifies \( t_n(\bar{r}, \bar{v}) = 0 \) on the absorbing boundary \( (\bar{r} \in \Sigma) \), for all \( n \geq 1 \) and for an outward velocity. Noting that the symmetric quantity \( \int d\bar{v} \int d\bar{v}' t_n(\bar{r}, \bar{v}') - \int d\bar{v} \int d\bar{v}' [t_n(\bar{r}, \bar{v})] \) obviously equals zero, and that \( \bar{v} \cdot \nabla_{\bar{r}} t_n(\bar{r}, \bar{v}) = \text{div}(t_n(\bar{r}, \bar{v})\bar{v}) \), the integration of eq. (3) over all possible initial positions and velocities gives

\[
\int d\bar{v} \int_V d\bar{v} \text{div}(t_n(\bar{r}, \bar{v})\bar{v}) = -n \int d\bar{v} \int_V d\bar{v} t_{n-1}(\bar{r}, \bar{v}).
\]

Applying the Gauss divergence theorem on the left-hand side of eq. (4), we can write that

\[
\langle t_n \rangle_{\Sigma} = \eta_d \frac{n V}{\bar{v} \Sigma} \langle t_{n-1} \rangle_V,
\]

where the two averages involved in eq. (5) are defined for any function \( f \) as follows:

\[
\langle f \rangle_{\Sigma} = -\frac{1}{v \Sigma \alpha_d} \int d\bar{v} \int_{\Sigma} d\bar{v}' \bar{v} f(\bar{r}, \bar{v}), \quad \text{and} \quad \langle f \rangle_V = \frac{1}{V \sigma_d} \int d\bar{v} \int_V d\bar{v} f(\bar{r}, \bar{v})
\]

with \( \alpha_d = \frac{2\pi^{\frac{d-1}{2}}}{(d-1)\Gamma(\frac{d-1}{2})} \) is the inward flux of a unit, isotropically distributed vector through a unit surface, and \( \eta_d = \frac{\alpha_d}{\sqrt{\pi} \sigma_d} \Gamma(\frac{d-1}{2}) \) is a dimension-dependent constant. Equation (5) can be rewritten as

\[
\langle t_1 \rangle_{\Sigma} = \eta_d \frac{V}{\bar{v} \Sigma}, \quad \text{and} \quad \forall n \geq 1, \quad \langle t_{n-1} \rangle_V = \frac{\langle t_n \rangle_{\Sigma}}{n \langle t_1 \rangle_{\Sigma}}
\]
Fig. 1 – A particular particle's trajectory which starts and ends on the absorbing boundary \( \Sigma_{abs} \), for an absorbing region inside a closed reflecting surface \( \Sigma \).

Fig. 2 – A particular particle's trajectory for a reflecting box with a hole (aperture) \( \Sigma_{abs} \).

which corresponds to the results previously obtained by Blanco and Fournier [1] and Mazzolo [5]. Parenthetically, we know that since \( \langle t_2 \rangle_{\Sigma} \geq \langle t_1 \rangle_{\Sigma}^2 \), (7) yields a general lower bound for \( \langle t_1 \rangle_{V} \):

\[
\langle t_1 \rangle_{V} \geq \frac{1}{2} \langle t_1 \rangle_{\Sigma} = \frac{\eta_d V}{2v_{\Sigma}}.
\]

(8)

General boundary conditions. – We now extend these results, which take unexpected simple forms, to the general case of mixed boundary conditions. The domain’s boundary \( \Sigma \) is now supposed to be composed of any combination of absorbing and reflecting parts (see figs. 1, 2). Let \( \Sigma_{abs} \) be the absorbing part of \( \Sigma \), and \( \Sigma_{refl} \) its reflecting part, so that \( \Sigma = \Sigma_{abs} + \Sigma_{refl} \). We assume that initially the particle starts from the absorbing surface. Whether we consider that the reflecting boundary is perfect, i.e. that the inward velocity angle equals the outward velocity angle, or whether we consider that the particle’s velocity angle is uniformly redistributed after each collision with the reflecting boundary, we have

\[
\int d\tilde{v} \int_{\Sigma_{refl}} d\Sigma \cdot \tilde{v} \ell_n(\tilde{r}, \tilde{v}) = 0.
\]

(9)

In this case of mixed boundary conditions, eq. (7) becomes

\[
\langle t_1 \rangle_{\Sigma_{abs}} = \frac{\eta_d V}{v_{\Sigma_{abs}}}, \quad \text{and} \quad \forall n \geq 1, \quad \langle t_{n-1} \rangle_{V} = \frac{\langle t_n \rangle_{\Sigma_{abs}}}{n \langle t_1 \rangle_{\Sigma_{abs}}}. \]

(10)

Let us, for instance, consider animals leaving their home through its boundary \( \Sigma_{abs} \), and exploring a domain \( V \) (see fig. 1). The previous equation gives a simple estimate of their mean return time to home if the boundary \( \Sigma_{refl} \) is reflecting for them, provided that the interrupted ballistic motion correctly models their behaviour.

Splitting probabilities. – Consider now a closed volume \( V \) with two absorbing surfaces \( \Sigma_1 \) and \( \Sigma_2 \), and let us compute the absorption probability \( \Pi_1(\tilde{r}, \tilde{v}) \) on the surface \( \Sigma_1 \) for a particle starting initially from the boundary \( \Sigma_{abs} = \Sigma_1 + \Sigma_2 \). This probability obeys the differential equation [8]

\[
\tilde{v} \cdot \nabla_\tilde{r} \Pi_1(\tilde{r}, \tilde{v}) + \frac{\lambda}{\sigma_d} \int d\tilde{v}' \left[ \Pi_1(\tilde{r}, \tilde{v}') - \Pi_1(\tilde{r}, \tilde{v}) \right] = 0,
\]

(11)
for which the boundary conditions, for an outward velocity $\vec{v}$, are $\Pi_1(\vec{r}, \vec{v})_{\vec{r} \in \Sigma_1} = 1$ and $\Pi_1(\vec{r}, \vec{v})_{\vec{r} \in \Sigma_2} = 0$. Following the same lines as previously, one can show that

$$\langle \Pi_1 \rangle_{\Sigma_{\text{abs}}} = \frac{\Sigma_1}{\Sigma_1 + \Sigma_2}. \quad (12)$$

In other words, the splitting probability through absorbing boundary is uniform, when starting uniformly from any point of it.

Residence time. – A relevant quantity involved in the theory of chemical reactivity and in other similar problems [9–12] is the residence time in a sub-domain $V'$ of the volume $V$. In order to study it, we assume that the particle can disappear in $V'$ (but not outside $V'$) with a constant and uniform reaction rate $k$. The central quantity is now the survival probability of the particle with respect to the reaction in volume $V'$ (i.e. considering that an absorption on the boundary is not a killing process), which can be expressed in two ways [12–14]:

$$S(t|\vec{r}, \vec{v}) = \int d\vec{r}' d\vec{v}' p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}) = \langle e^{-kT_t(\vec{r}, \vec{v})} \rangle, \quad (13)$$

where $T_t$ is the residence time up to the observation time $t$ inside $V'$ of the particle, starting from $(\vec{r}, \vec{v})$, and $p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v})$ is the conditional density probability of the particle which satisfies the following backward Chapman-Kolmogorov differential equation:

$$\partial_t p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}) = \vec{v}' \cdot \vec{\nabla}_{\vec{r}'} p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}) + \frac{\lambda}{\sigma_d} \int d\vec{v}'' [p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}'') - p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v})] - k \mathbf{1}_{V'}(\vec{r}') p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}), \quad (14)$$

where $\mathbf{1}_{V'}(\vec{r})$ is the indicator function of $V'$ which equals zero if $\vec{r} \notin V'$ and equals one if $\vec{r} \in V'$. Note that the boundary conditions give $S(t|\vec{r}, \vec{v}) = 1$ for an outward velocity of a particle on the absorbing surface $\Sigma_{\text{abs}}$. Indeed, such a particle absorbed on this surface will never disappear within the sub-domain $V'$. Writing down eq. (14) for the conditional survival probability, we obtain

$$\partial_t S(t|\vec{r}, \vec{v}) = \vec{v} \cdot \vec{\nabla}_{\vec{r}} S(t|\vec{r}, \vec{v}) + \frac{\lambda}{\sigma_d} \int d\vec{v}' [S(t|\vec{r}, \vec{v}')] - S(t|\vec{r}, \vec{v})] - k \mathbf{1}_{V'}(\vec{r}) S(t|\vec{r}, \vec{v}). \quad (15)$$

As $S(t|\vec{r}, \vec{v})$ is a bounded non-increasing function of $t$, it tends to a finite limit as $t \to \infty$, so much $\frac{\partial S}{\partial t} \to 0$. Letting $t \to \infty$ in (15), integrating it over $\vec{r} \in V$ and $\vec{v}$, taking into account
the boundary conditions and using the expansion (see (13) when \( t \to \infty \))

\[
S_\infty(\vec{r}, \vec{v}) = \sum_{n=0}^{+\infty} (-1)^n \frac{k^n}{n!} \tau_n(\vec{r}, \vec{v}),
\]

(16)

where \( \tau_n(\vec{r}, \vec{v}) \) is the \( n \)-th moment of the residence time of the particle inside \( V' \) for an infinite observation time, we derive our main result for the residence time:

\[
\langle \tau_1 \rangle_{\text{abs}} = \frac{\eta d}{v} \frac{V'}{\Sigma_{\text{abs}}}, \quad \text{and} \quad \forall n \geq 1, \quad \langle \tau_{n-1} \rangle_{\text{abs}} = \frac{\langle \tau_n \rangle_{\text{abs}}}{n \langle \tau_1 \rangle_{\text{abs}}}. \]

(17)

Note that the mean fraction of time spent inside \( V' \) prior to the first exit of \( V \) is given by \( \langle \tau_1 \rangle_{\text{abs}}/\langle t_1 \rangle_{\text{abs}} = V'/V \), which can be seen as an ergodic-type property [8].

**Generalisation.** – Let us now assume that the particle undergoes a more general stochastic diffusion process, interrupted at stochastic times by an instantaneous redistribution of its velocity, without changing its position. The conditional density probability \( p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}) \) to be at position \( \vec{r}' \) with velocity \( \vec{v}' \) at time \( t \), starting from \( (\vec{r}, \vec{v}) \) at time 0, corresponding to the general diffusion process obeys the backward equation

\[
\partial_t p = v_i \partial_{x_i} p + \frac{F_i}{m} \partial_{v_i} p + D_{ij} \partial_{v_i v_j}^2 p \equiv L^+ p,
\]

(18)

where \( m \) is the mass of the particle, \( \vec{F}(\vec{r}, \vec{v}) \) is the force exerted on the particle in state \( (\vec{r}, \vec{v}) \), \( D_{ij} \) is the general diffusion matrix, and \( L^+ \) stands for the adjoint of \( L \). In many situations of physical interest, \( \vec{F} \) is the sum of a conservative force due to a potential \( U \), \( -\partial_t U \), and of a friction force \( -\eta \vec{v} \) due to a surrounding fluid, \( \eta \) being a constant friction coefficient. Furthermore, \( D_{ij} = \delta_{ij} D \eta^2 / m^2 \), \( D \) being the usual diffusion coefficient of the Fick law, which is independent of \( \vec{r} \) in a homogeneous medium. Now, we assume that this general diffusion process is interrupted at stochastic times, for which the velocity \( \vec{v} \) of the particle is instantaneously redistributed with a given transition rate \( q(\vec{r}, \vec{v}'|\vec{r}, \vec{v}) \). The overall stochastic process, including the velocity reorientation, obeys the equation

\[
\partial_t p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}) = L^+ p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}) + \int d\vec{v}'' q(\vec{r}', \vec{v}'|\vec{r}, \vec{v}) \left[ (p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}'') - p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v})) \right]
\]

\[
\equiv L^+ p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}).
\]

(19)

The conditional probability density at time \( t \), \( p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}) \) also obeys the following forward equation:

\[
\partial_t p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}) = L p(\vec{r}', \vec{v}', t|\vec{r}, \vec{v}).
\]

(20)

Let us assume that this equation, when the whole boundary \( \Sigma \) is assumed to be reflecting, admits a stationary solution \( p_0(\vec{r}, \vec{v}) \). For instance, \( p_0(\vec{r}, \vec{v}) \) is the thermodynamic equilibrium \( \propto e^{-(U + \frac{\vec{v}^2}{2m})/k_B T} \) if eq. (18) is the usual diffusion equation of a particle in an equilibrium fluid at temperature \( T \) and if the velocity redistribution process defined previously does not affect this thermodynamic equilibrium, which is the case if \( \int d\vec{v}'' q(\vec{r}, \vec{v}'|\vec{r}, \vec{v}) p_0(\vec{r}, \vec{v}) - q(\vec{r}, \vec{v}'|\vec{r}, \vec{v}'') p_0(\vec{r}, \vec{v}'') \) = 0. Then it is possible to generalize the previous results. Indeed, let us consider the residence time of the particle in a sub-domain \( V' \subset V \), and let \( \Sigma_{\text{abs}} \) be the absorbing part of the total surface \( \Sigma \). As previously, we assume that inside \( V' \), the particle can
disappear with a constant and uniform reaction rate \( k \). Its conditional survival probability at time \( t \), \( S(t|\vec{r}, \vec{v}) = \int d\vec{r} d\vec{v} p(\vec{r}, \vec{v}, t|\vec{r}, \vec{v}) \), starting from \((\vec{r} \in V, \vec{v})\) obeys the backward equation

\[
\frac{\partial}{\partial t} S(t|\vec{r}, \vec{v}) = \mathcal{L}^+ S(t|\vec{r}, \vec{v}) - k \mathbf{1}_{V'}(\vec{r}) S(t|\vec{r}, \vec{v}),
\]

(21)

where \( \mathbf{1}_{V'}(\vec{r}) = 1 \) if \( \vec{r} \in V' \) and 0 otherwise. Following the method used for the Pearson random walks, we let \( t \to +\infty \) in (21), and we multiply this equation by the equilibrium probability \( p_0(\vec{r}, \vec{v}) \) computed for the reflecting conditions on the boundary \( \Sigma \) of \( V \). The integration of eq. (21) over all \( \vec{r} \in V \) and \( \vec{v} \) leads to

\[
\int_{\vec{r} \in V} d\vec{r} \int d\vec{v} p_0(\vec{r}, \vec{v}) \mathcal{L}^+ S_\infty(\vec{r}, \vec{v}) = k \int_{\vec{r} \in V'} d\vec{r} \int d\vec{v} p_0(\vec{r}, \vec{v}) S_\infty(\vec{r}, \vec{v}).
\]

(22)

The left-hand side of (22) can be transformed into

\[
\int_{\vec{r} \in V} d\vec{r} \int d\vec{v} S_\infty(\vec{r}, \vec{v}) \mathcal{L} p_0(\vec{r}, \vec{v}) + \int_{\vec{r} \in \Sigma} d\vec{\Sigma} \cdot \vec{d} \vec{v} p_0(\vec{r}, \vec{v}).
\]

(23)

The first integral vanishes, since \( \mathcal{L} p_0(\vec{r}, \vec{v}) = 0 \) if \( \vec{r} \in V \). In the second integral we separate the inward and outward integration over \( \vec{v} \) in the surface integral. The inward part can be written, using the expansion (16) of \( S_\infty \): \( \sum_{n=0}^\infty (-1)^n n! J(\tau_n) \Sigma_{\text{abs}} \), where \( J = -\int_{\vec{r} \in \Sigma_{\text{abs}}} d\vec{\Sigma} \). The one-way equilibrium probability current on \( \Sigma_{\text{abs}} \), and the surface average of a quantity \( f(\vec{r}, \vec{v}) \) is defined as

\[
\langle f \rangle_{\Sigma_{\text{abs}}} = -\frac{1}{J} \int_{\vec{r} \in \Sigma_{\text{abs}}} d\vec{\Sigma} \cdot \int_{\vec{v}_n} d\vec{v} f(\vec{r}, \vec{v}) p_0(\vec{r}, \vec{v}).
\]

(24)

The outward part is actually equal to \( J \), as \( S_\infty(\vec{r}, \vec{v}) = 1 \) if \( \vec{r} \in \Sigma \) and \( \vec{v} \) points outward. Then, comparing both sides of (22), we generalize relations (17) for the moments of the residence time within \( V' \):

\[
\langle \tau_1 \rangle_{\Sigma_{\text{abs}}} = \frac{P}{J} \quad \text{and} \quad \langle \tau_n \rangle_{\Sigma_{\text{abs}}} = n \frac{\langle \tau_{n-1} \rangle_{V'}}{J},
\]

(25)

where \( P = \int_{\vec{r} \in V'} d\vec{r} d\vec{v} p_0(\vec{r}, \vec{v}) \) is the equilibrium probability of volume \( V' \).

Considering now the special case \( V' = V \), we obtain the relations for the moments of the first exit time from \( V \):

\[
\langle t_1 \rangle_{\Sigma_{\text{abs}}} = \frac{1}{J} \quad \text{and} \quad \langle t_{n-1} \rangle_V = \frac{1}{n} \langle t_n \rangle_{\Sigma_{\text{abs}}},
\]

(26)

which generalize formulas (7). In the same way, the results of the splitting probabilities (12) can be generalized for the general stochastic motion discussed here. Equation (26) takes a particularly simple form if we now consider a fluid of identical particles and if we replace \( p_0(\vec{r}, \vec{v}) \) by the equilibrium density of particles in the phase space \((\vec{r}, \vec{v})\). Then, the probability current \( J \) is replaced by the equilibrium one-way flux of particles \( \phi \) through \( \Sigma \), and eq. (26) becomes

\[
\langle t_1 \rangle_{\Sigma} = \frac{N}{\phi},
\]

(27)

\( N \) being the number of particles in \( V \). This formula can easily be understood intuitively: if at time 0 the boundary is supposed to be reflecting, the number of particles leaving \( V \) per unit time should be \( \sim \frac{1}{\langle t_1 \rangle_{\Sigma}} \), so that the equilibrium is maintained inside \( V \) if \( V \) is supplied with an entering flux of new particles \( \phi \sim \frac{N}{\langle t_1 \rangle_{\Sigma}} \).
**Conclusion.** – We have shown that the geometrical relations previously obtained for Pearson random walks in bounded domains are particular cases of very general relations between residence times for a large class of stochastic processes. Thus, they can be very useful in many applications, when the evolution equations cannot be solved exactly. Furthermore they can be extended to intermittent systems, which are frequent in biology [15]. Lastly, with relevant changes, this work can be extended to discrete space and time systems. Such extensions are in progress.

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We thank S. CONDAMIN for useful discussions.

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