

Occupation times for single-file diffusion

Olivier Bénichou, Jean Desbois

▶ To cite this version:

Olivier Bénichou, Jean Desbois. Occupation times for single-file diffusion. Journal of Statistical Mechanics: Theory and Experiment, 2015, pp.P03001. hal-01135431

HAL Id: hal-01135431 https://hal.science/hal-01135431

Submitted on 25 Mar 2015

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Home Search Collections Journals About Contact us My IOPscience

Occupation times for single-file diffusion

This content has been downloaded from IOPscience. Please scroll down to see the full text.

J. Stat. Mech. (2015) P03001

(http://iopscience.iop.org/1742-5468/2015/3/P03001)

View the table of contents for this issue, or go to the journal homepage for more

Download details:

IP Address: 129.175.97.14 This content was downloaded on 25/03/2015 at 11:20

Please note that terms and conditions apply.

J. Stat. Mech. (2015) P03001



Occupation times for single-file diffusion

Olivier Bénichou¹ and Jean Desbois²

 1 Laboratoire de Physique Théorique de la Matière Condensée (UMR CNRS 7600), Université Pierre et Marie Curie, 4 Place Jussieu, 75255 Paris Cedex, France

² Laboratoire de Physique Théorique et Modèles Statistiques (UMR CNRS 8626), Université Paris-Sud, 91405 Orsay, France
E-mail: benichou@lptmc.jussieu.fr and desbois@lptms.u-psud.fr

Received 12 December 2014 Accepted for publication 30 January 2015 Published 3 March 2015

Online at stacks.iop.org/JSTAT/2015/P03001 doi:10.1088/1742-5468/2015/03/P03001

Abstract. We consider a file of identical Brownian particles moving on the same axis x'Ox without crossing each other. They all start from the origin O at time t = 0 and are stopped at some time t. Denoting by T the time spent on the half-line [Ox) by a given particle of the line, we establish analytical formulae for the first two moments $\langle T \rangle$ and $\langle T^2 \rangle$. In particular, considering the limit of an infinite number of particles, we get, for the 'middle' particle

$$\left\langle \left(\frac{T}{t}\right)^2 \right\rangle = \frac{3}{8} + \frac{1}{8}J_0(\pi) = 0.336\,96...$$

 $(J_0 \text{ is a Bessel function})$. This result (and also numerical simulations) shows that the distribution of T, though being close to it, is not fully a constant one.

Keywords: stochastic processes (theory), Brownian motion, diffusion

Contents

1.	Introduction	2
2.	Basic setup	4
3.	Occupation time of the middle particle (rank $l = q + 1$) of a file of $n = 2q + 1$ particles 3.1. The three particle case $(q = 1)$ 3.2. General q values 3.3. The limit $q \to \infty$.	4 4 6 7
4.	Occupation time of a particle of general rank l 4.1. The first moment $\langle u \rangle$	9 10
	4.2.1 The second moment (a^{\prime}) 4.2.1. The three particle case	11 12
5.	4.2.1 The second moment (a^{-}) 4.2.1. The three particle case. 4.2.2. The limit $q \to \infty$.	10 11 12 13

1. Introduction

Single file diffusion is defined as the diffusion of a tracer particle in a one dimensional system of hard-core Brownian particles. This type of model is used in many physical, chemical, and biological processes to analyze the dynamics of particles in crowded quasidimensional systems. Experimentally, it has been evidenced by passive microrheology in zeolites, transport of confined colloidal particles, or charged spheres in circular channels [1– 4]. Due to the hard-core interactions, the order of particles is unchanged with time, which results when infinitely many hard-core particles are present in a subdiffusive behavior of the mean-square displacement of the tracer particle $\langle X_t^2 \rangle \propto \sqrt{t}$. This result, first discovered analytically by Harris [5], has been extended in several directions, both for discrete and continuous variants of the model. Examples include the determination of the full propagator for the tracer particle [6], the treatment of the case where the motion of the bath particles is subdiffusive [7], the case where the tracer particle performs a biased diffusion [8] or the determination of first-passage properties [9]. In contrast, the analysis of occupation times for single file diffusion—the cumulative time spent by the tracer particle on the positive half-line up to a given observation time—does not seem to have been considered so far.

Let us first recall that the study of occupation times for an *isolated* Brownian motion (BM) traces back to the famous Levy's arc-sine law [10, 11]. It states that, for a

one-dimensional Brownian motion (BM(\mathbb{R})) starting at the origin at t = 0 and stopped at t, the time T spent when x > 0 satisfies the probability law ($0 < t_1 < t$):

$$P(T < t_1) = \frac{2}{\pi} \arcsin \sqrt{\frac{t_1}{t}}$$
(1)

with the symmetric U-shape density:

$$\mathcal{P}(T) = \frac{1}{\pi} \frac{1}{\sqrt{T(t-T)}} \tag{2}$$

Barlow, Pitman and Yor [12] have extended Levy's result to a BM on a set of n semiinfinite lines originating from O (a kind of special graph). $\{T_i\}$ being the set of occupation times on all the lines, the authors computed explicitly the Laplace transform of the $\{T_i\}$ distribution. This study has itself been extended more recently [13] to a BM on a quite general graph. A step further was done in [14] where the exit and occupation times were studied, still on graphs, for a BM with general drift and boundary conditions.

On another hand, thoretical physicists [15] and also mathematicians [16] were interested in the quadrant occupation time T for the planar BM. In particular, the first four moments of this occupation time are computed in [15], with the result³:

$$\left\langle \left(\frac{T}{t}\right)\right\rangle = \frac{1}{4} \tag{3}$$

$$\left\langle \left(\frac{T}{t}\right)^2 \right\rangle = \frac{5}{32} - \frac{1}{8\pi^2} = 0.14358... \approx \frac{1}{7}$$
 (4)

$$\left\langle \left(\frac{T}{t}\right)^3 \right\rangle = \frac{63}{512} - \frac{7}{32\pi^2} = 0.100\,88... \approx \frac{1}{10}$$
 (5)

$$\left\langle \left(\frac{T}{t}\right)^4 \right\rangle = \frac{907}{8192} - \frac{1}{64\pi} - \frac{631}{2304\pi^2} - \frac{7}{384\pi^4} = 0.0778... \approx \frac{1}{13}$$
(6)

Despite the importance of the problem, the determination of occupation times for single file diffusion does not seem to have been investigated so far. Here we consider hard-core one-dimensional Brownian particles that all start from the origin O at time t = 0 and are stopped at some time t. We will be interested in the time T spent on the half-line [Ox) by a given particle of the line, both for a finite and infinite number of Brownian particles. Note that, while the evolution of the full system is Markovian, the dynamics of the only tracer is not. These memory effects make the determination of the occupation time T a non-trivial problem. Here, we focus on the two first moments $\langle T \rangle$ and $\langle T^2 \rangle$.

The outline of the paper is more precisely as follows. We first define the dynamics of the system and show that the determination of the occupation time of a given particle of the line can be mapped onto a single particle problem. We next consider the particular case when the tracer particle is the 'middle' particle of the line. Analytical formulae for the two first moments of the occupation time are derived for an arbitrary (odd) number of particles on the line. The limit of an infinite number of particles is then analyzed in detail. Finally, these results are extended to the case of a tracer of arbitrary position in the line.

³ Equation (2) is the beta law $B_{1/2,1/2}$. It is worth noticing that, despite the complication of the results equations (3)–(6), those moments are very close to the ones of the beta law $B_{1,1/3}$ that are, respectively, $\frac{1}{4}$, $\frac{1}{7}$, $\frac{1}{10}$, $\frac{1}{13}$. We will come back to those results in section 4.

2. Basic setup

We adopt here a continuous space description of the system and consider a file of n = 2q+1 identical Brownian particles p_l moving on a line x'Ox. Those particles are labelled by their rank l (= 1, 2, ..., 2q + 1) and cannot cross each other. l = 1 labels the rightmost particle, l = 2q + 1 the leftmost particle and l = q + 1 the 'middle' particle.

Two adjacent particles can experience elastic collisions. During such collisions, they simply exchange their velocities because they are identical. Alternatively, we can consider that the particles are free to cross each other, only exchanging their ranks at each collision. Pushing this picture further, we are left with a unique Brownian particle P, freely moving in \mathbb{R}^n , whose coordinates x_i represent the positions of the previous particles.

For the sake of simplicity, we will consider that P starts its motion at the origin at t = 0 and stops somewhere at time t. This implies, in particular, that, at t = 0, all the particles p_l are at the same point O. This could seem unrealistic because the particles are mutually impenetrable. Nevertheless we think this is not the case. Indeed, this is equivalent to supposing that at t = 0 the particles are well separated (but chosen arbitrarily close to their neighbours because they are all point-like) and that we stop the motion at sufficiently large t.

We are interested in the time T spent by the particle of rank l on the half line x > 0. T is equal to the time spent by P in all the orthants of \mathbb{R}^n with, **at least**, l positive coordinates. From general scaling properties of the Brownian motion starting from O, we deduce that T scales like t and define⁴ the random variable $u = \frac{T}{t}$. In the following, we will be especially interested in the computation of the first two moments of u.

3. Occupation time of the middle particle (rank l = q + 1) of a file of n = 2q + 1 particles

3.1. The three particle case (q = 1)

Let us first consider the particular case of three particles and show how $\langle T^2 \rangle$ can be computed for the rank 2 particle.

Following the previous section, we consider a particle P freely wandering in \mathbb{R}^3 . Among the 2^3 orthants in \mathbb{R}^3 , only four of them will be relevant for the computation of the moments⁵ $\langle T^k \rangle$: $(x_1, x_2, x_3 > 0) \equiv \mathcal{U}_1$, $(x_1, x_2 > 0, x_3 < 0) \equiv \mathcal{U}_2$, $(x_1 > 0, x_2 < 0, x_3 > 0) \equiv \mathcal{U}_3$, $(x_1 < 0, x_2, x_3 > 0) \equiv \mathcal{U}_4$. Let us call \mathcal{U} the sum of these four orthants.

The moments $\langle T^k \rangle$ are given by an expansion of the following identity in powers of λ :

$$\langle e^{-\lambda T} \rangle = \int_{\mathbb{R}^3} d^3 \overrightarrow{r} \left\langle \overrightarrow{r} | e^{-H_{\lambda} t} | \overrightarrow{0} \right\rangle$$
 (7)

where

 $e \qquad H_{\lambda}(\overrightarrow{r}) = -\frac{1}{2}\Delta + \lambda \ \mathbf{1}_{\mathcal{U}}(\overrightarrow{r}) \tag{8}$

 $(1_{\mathcal{U}}(\overrightarrow{r}) = 1 \text{ if } \overrightarrow{r} \in \mathcal{U}, = 0 \text{ otherwise}).$

 4 We will see that the random variable u appears naturally in the following computations.

⁵ We immediately deduce the obvious result $\langle u \rangle = 1/2$ for the middle particle.

Occupation times for single-file diffusion

The second order in λ leads to:

$$\left\langle \left(\frac{T^2}{2}\right) \right\rangle = \int_0^t dt_2 \int_0^{t_2} dt_1 \int_{\mathcal{U}} dx_1 dx_2 dx_3 \int_{\mathcal{U}} dx'_1 dx'_2 dx'_3 \\ \times \mathcal{G}(x_1, x_2, x_3; t_1) \mathcal{G}(x'_1 - x_1, x'_2 - x_2, x'_3 - x_3; t_2 - t_1)$$
(9)

where \mathcal{G} is the 3D-propagator:

$$\mathcal{G}(x_1, x_2, x_3; t) = G(x_1; t)G(x_2; t)G(x_3; t)$$
(10)

with
$$G(x;t) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{x^2}{2t}\right)$$
 (11)

Writing the spatial integral

$$\int_{\mathcal{U}} dx_1 dx_2 dx_3 \int_{\mathcal{U}} dx_1' dx_2' dx_3' \mathcal{G}(x_1, x_2, x_3; t_1) \mathcal{G}(x_1' - x_1, x_2' - x_2, x_3' - x_3; t_2 - t_1)$$

as $\int_{\mathcal{U}} \int_{\mathcal{U}} \mathcal{G} \mathcal{G}$, we get, with standard manipulations:

$$\int_{\mathcal{U}} \int_{\mathcal{U}} \mathcal{G} \mathcal{G} = \left(4 \int_{\mathcal{U}_1} \int_{\mathcal{U}_1} + 6 \int_{\mathcal{U}_1} \int_{\mathcal{U}_2} + 6 \int_{\mathcal{U}_2} \int_{\mathcal{U}_3} \right) \mathcal{G} \mathcal{G}$$
(12)

Now, let us introduce the integrals $\sim \sim \sim$

$$J = \int_{0}^{\infty} dx \int_{0}^{\infty} dx' G(x; t_1) G(x' - x; t_2 - t_1) = \frac{1}{4} + \frac{1}{2\pi} \arcsin\sqrt{\frac{t_1}{t_2}} \equiv \frac{1}{4\pi} (\pi + \phi)$$
(13)

$$J' = \int_{0}^{\infty} \mathrm{d}x \int_{-\infty}^{0} \mathrm{d}x' G(x;t_1) G(x'-x;t_2-t_1) = \frac{1}{4} - \frac{1}{2\pi} \arcsin\sqrt{\frac{t_1}{t_2}} \equiv \frac{1}{4\pi} (\pi - \phi)$$
(14)

where we have set $\frac{t_1}{t_2} = \sin^2(\phi/2)$. It is worth noticing that a factor $(\pi + \phi)$ is generated when xx' > 0 and $(\pi - \phi)$ when xx' < 0.

So, we can immediately write:

$$\int_{\mathcal{U}_1} \int_{\mathcal{U}_1} \mathcal{G} \mathcal{G} = J^3 \tag{15}$$

$$\int_{\mathcal{U}_1} \int_{\mathcal{U}_2} \mathcal{G} \mathcal{G} = J^2 J' \tag{16}$$

$$\int_{\mathcal{U}_2} \int_{\mathcal{U}_3} \mathcal{G} \mathcal{G} = J J'^2 \tag{17}$$

Finally, we get:

$$\left\langle \left(\frac{T^2}{2}\right) \right\rangle = \frac{t^2}{2} \int_0^{\pi} \mathrm{d}\phi \frac{\sin\phi}{2(4\pi)^3} \left(4(\pi+\phi)^3 + 6(\pi+\phi)^2(\pi-\phi) + 6(\pi+\phi)(\pi-\phi)^2\right)$$
(18)

$$\langle u^2 \rangle = \frac{3}{8} - \frac{3}{16\pi^2} = 0.356\,00...$$
 (19)

Recall that for a single particle (q = 0), we should have $\langle u^2 \rangle = \frac{3}{8} = 0.375$. We observe that, for the middle particle, $\langle u^2 \rangle$ decreases when *n* increases from 1 to 3. We will come back to this point later in section 4.2.1.

Occupation	times	for	single-file	diffusion
Occupation	LIIIICS	101	single-me	unnusion

q	n	l	$\langle u^2 \rangle$
0	1	1	$\frac{3}{8} = 0.375$
1	3	2	$\frac{3}{8} - \frac{3}{16\pi^2} = 0.35600\dots$
2	5	3	$\frac{3}{8} - \frac{15}{32\pi^2} + \frac{135}{64\pi^4} = 0.34916$
3	7	4	$\frac{3}{8} - \frac{105}{128\pi^2} + \frac{735}{64\pi^4} - \frac{7875}{128\pi^6} = 0.34578\dots$
7	15	8	0.34101
50	101	51	0.337 53

Table 1. The second moment, $\langle u^2 \rangle$, for the middle particle of a file of *n* particles.

3.2. General q values

We now extend the previous results to the case of an arbitrary (odd) number of particles in the file. Following the previous section 3.1, we have to consider two positions of the particle P with, at least, (q+1) positive coordinates and we must distinguish the coordinates that will keep their sign from the other ones. More precisely, we consider the configuration built with:

- (a) a first position with (m + k) negative coordinates
- (b) a second position with (m+r) negative coordinates

such that m coordinates will stay negative and (k+r) will change of sign. So, 2q+1-(k+r) coordinates will keep their sign. The contribution of such a configuration to $\langle u^2 \rangle$ will be equal to:

$$\frac{1}{2(4\pi)^{2q+1}} \int_{0}^{\pi} \mathrm{d}\phi \,\sin\phi \,(\pi+\phi)^{2q+1-k-r}(\pi-\phi)^{k+r}$$

Now, the number of configurations with given m, k, r is simply $\frac{(2q+1)!}{m!k!r!(2q+1-m-k-r)!}$. Observing that $m + k \leq q$ and $m + r \leq q$, we get the general expression for $\langle u^2 \rangle$:

$$\left\langle u^{2} \right\rangle = \frac{1}{2(4\pi)^{2q+1}} \int_{0}^{\pi} \mathrm{d}\phi \sin\phi \sum_{m=0}^{q} \sum_{k=0}^{q-m} \sum_{r=0}^{q-m} \frac{(2q+1)!(\pi+\phi)^{2q+1-k-r}(\pi-\phi)^{k+r}}{m!k!r!(2q+1-m-k-r)!}$$
(20)

The results for different q values are quoted in table 1.

We observe that $\langle u^2 \rangle$ is written as a series in $\frac{1}{\pi^2}$ starting with the term $\frac{3}{8}$. Moreover, $\langle u^2 \rangle$ decreases when q increases and seems to have a limit close to $\frac{1}{3}$ that could be consistent with a constant distribution $P_{q+1}(u)$. The same indication comes out from numerical simulations that show that this distribution becomes flatter and flatter as long as q increases (see figure 1 where the integrated probability density $F_{q+1}(u) = \int_0^u P_{q+1}(v) \, dv$ is plotted). All those considerations motivate us to study the limit of $\langle u^2 \rangle$ when $q \to \infty$.

Occupation times for single-file diffusion



Figure 1. The evolution of the integrated distribution $F_{q+1}(u)$ for the middle particle when the number of particles in the file increases. Numerical simulations $(5 \times 10^6 \text{ events}, 5 \times 10^5 \text{ gaussian steps})$ for (a) a single particle (q = 0): + (the curve is the arc-sine law); (b) a file of three particles (q = 1): ×; (c) a file of 11 particles (q = 5): *. (In (b) and (c), the lines are drawn to guide the eye.) In (d), we display (dotted line) the diagonal $F_{q+1}(u) = u$ that should appear for a flat distribution $P_{q+1}(u) = 1$.

3.3. The limit $q \rightarrow \infty$

To study $\langle u^2 \rangle$ in that limit, we first set: $m \equiv qX$, $k \equiv qY$, $r \equiv qZ$, and write the summations in equation (20) as integrals:

$$\sum_{m=0}^{q} \sum_{k=0}^{q-m} \sum_{r=0}^{q-m} \frac{(2q+1)!(\pi+\phi)^{2q+1-k-r}(\pi-\phi)^{k+r}}{m!k!r!(2q+1-m-k-r)!} \approx q^{3} \int_{0}^{1} \mathrm{d}X \int_{0}^{1-X} \mathrm{d}Y \int_{0}^{1-X} \mathrm{d}Z \exp(I(X,Y,Z))$$
(21)

The integration domain \mathcal{D} is displayed in figure 2(a): we integrate inside the pyramid AOCBD.

Now, using the Stirling formula, we apply the saddle-point method (ϕ is fixed). With the conditions

$$\frac{\partial I}{\partial X}\Big|_{X_0, Y_0, Z_0} = \frac{\partial I}{\partial Y}\Big|_{X_0, Y_0, Z_0} = \frac{\partial I}{\partial Z}\Big|_{X_0, Y_0, Z_0} = 0$$

we get the saddle-point $M_0(X_0, Y_0, Z_0)$ that lies between A and B (see figure 2(a)):

$$X_0 = \frac{1}{2} + \frac{\phi}{2\pi}$$
(22)

$$Y_0 = Z_0 = \frac{1}{2} - \frac{\phi}{2\pi} = 1 - X_0 \tag{23}$$

$$\exp(I(X_0, Y_0, Z_0)) = \frac{(4\pi)^{2q+1} 2\sqrt{\pi}}{q^{3/2} (\pi - \phi)(\pi + \phi)}$$
(24)





Figure 2. (a) The integration domain \mathcal{D} —the interior of the pyramid AOCBD, the saddle-point M_0 and the three perpendicular axes $\overline{M_0X'}, \overline{M_0Y'}, \overline{M_0Z'};$ (b) the integration domain \mathcal{D}' .

Then,
$$\langle u^2 \rangle$$
 is written as:

$$\left\langle u^2 \right\rangle = \sqrt{\pi} q^{3/2} \int_0^{\pi} \frac{\mathrm{d}\phi \sin \phi}{(\pi - \phi)(\pi + \phi)} \int_{\mathcal{D}} \mathrm{d}X \mathrm{d}Y \mathrm{d}Z \exp(V) \tag{25}$$

$$V = -\frac{q}{X_0} \left((X - X_0)^2 + \frac{(Y - Y_0)^2 + (Z - Z_0)^2}{2(1 - X_0)} \right) - \frac{q}{X_0} \left((X - X_0)(Y - Y_0) + (X - X_0)(Z - Z_0) + (Z - Z_0)(Y - Y_0) \right)$$
(26)

Let us focus, for the moment, on the spatial (domain \mathcal{D}) integration.

Introducing (see figure 2(a)) the three perpendicular axes $(\overline{M_0X'}, \overline{M_0Y'}, \overline{M_0Z'})$ such that $\overline{M_0X'} \parallel \overrightarrow{BA}$ and such that $\overline{M_0Y'}$ lies in the plane Y = Z, we get:

$$V = -q \left(\frac{X'^2}{3X_0(1-X_0)} + \frac{(10-9X_0)Y'^2}{6X_0} + \frac{Z'^2}{2(1-X_0)} - \frac{2X'Y'}{3\sqrt{2}X_0(1-X_0)} \right)$$

q being large, we can perform the X' integration and get

$$\sqrt{\frac{3\pi X_0(1-X_0)}{q}} \times I'$$

where

$$I' \equiv \int_{\mathcal{D}'} dY' dZ' \exp\left(-q\left(\frac{3Y'^2}{2X_0} + \frac{Z'^2}{2(1-X_0)}\right)\right)$$
(27)

The integration domain \mathcal{D}' , for Y' and Z' is displayed in figure 2(b) (the angle between the two planes X + Y = 1 and X + Z = 1 is equal to $2\pi/3$).





Figure 3. Numerical simulations for a file of $21 \ (= 2q + 1)$ particles. The distribution $P_l(u)$ is displayed for the particles of ranks $9 \le l \le 13$. For l = 11 (middle particle), $P_l(u)$ still has a (flattened) symmetric U-shape. But $P_l(u)$ has a very different shape for the particles surrounding the middle one.

In the large q limit and using polar coordinates, we can compute

$$I' = \frac{2\sqrt{X_0(1-X_0)}}{q\sqrt{3}} \arcsin\sqrt{X_0}$$

Now, with the equations (22), (23) and (25), we get:

$$\left\langle u^2 \right\rangle = \frac{1}{2\pi} \int_0^\pi \mathrm{d}\phi \sin\phi \ \arcsin\sqrt{\frac{1}{2} + \frac{\phi}{2\pi}} \tag{28}$$

$$=\frac{1}{2\pi}\int_{0}^{\pi}\mathrm{d}\phi\sin\phi\left(\frac{\pi}{4}+\frac{1}{2}\arcsin\frac{\phi}{\pi}\right)$$
(29)

Finally, we obtain the analytical result for $q \to \infty$:

$$\langle u^2 \rangle = \frac{3}{8} + \frac{1}{8} J_0(\pi) = 0.336\,96...$$
 (30)

where J_0 is a standard Bessel function.

Interestingly, it is found that $\langle u^2 \rangle \neq \frac{1}{3}$. We thus conclude that the distribution of u is not constant.

4. Occupation time of a particle of general rank *I*

We now show that the previous results can be extended to determine the first two moments of the occupation time of a particle of arbitrary rank l.

Figure 3 displays the distribution $P_l(u)$ for different particles of rank l belonging to a file of n = 2q + 1 = 21 particles. We note that the shape of $P_l(u)$ is very sensitive to the value of l, especially for l close to 11 (= q + 1). We also remark that, obviously, $P_{10}(u) = P_{12}(1-u), P_9(u) = P_{13}(1-u), \dots$ and, more generally,

$$P_l(u) = P_{2q+2-l}(1-u) = P_{n+1-l}(1-u)$$
(31)

This reflects the symmetry with respect to the middle particle of the file. We will come back to this point later.

In the following, we will consider a particle of general rank l in a file of n = 2q + 1 particles⁶. In particular, we will focus our attention on the limit $q \to \infty$.

4.1. The first moment $\langle u \rangle$

To get $\langle u \rangle$, it is enough to count the number of orthants of \mathbb{R}^{2q+1} with, at least, l positive coordinates:

$$\langle u \rangle = \frac{\sum_{r=l}^{2q+1} \binom{2q+1}{r}}{2^{2q+1}}$$
(32)

With the Stirling formula and the replacement of the sum by an integral, we get, for large q values:

$$\langle u \rangle = \frac{1}{2} \operatorname{erfc}(a) \tag{33}$$

where erfc is the complementary error function:

$$\operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_{z}^{\infty} e^{-t^2} dt = 1 - \operatorname{erf}(z)$$
(34)

and

$$a = \sqrt{\frac{1}{q}} (l - (q+1)), \qquad 1 \le l \le 2q+1$$
 (35)

(a = 0 corresponds to the middle particle.)

As shown in figure 4(a), the agreement between equations (32) (for a file of n = 21 particles) and (33) is quite good.

4.2. The second moment $\langle u^2 \rangle$

Following the same lines as in section 3.2, we get the general result

$$\left\langle u^{2} \right\rangle = \frac{1}{2(4\pi)^{2q+1}} \int_{0}^{\pi} \mathrm{d}\phi \sin\phi \sum_{m=0}^{2q+1-l} \sum_{k=0}^{2q+1-l-m} \sum_{r=0}^{2q+1-l-m} \frac{(2q+1)!(\pi+\phi)^{2q+1-k-r}(\pi-\phi)^{k+r}}{m!k!r!(2q+1-m-k-r)!}$$
(36)

We remark that this expression is the same as equation (20) except for a change in the upper bounds of the summations; (20) is recovered when we set l = q + 1.

⁶ For *n* even, we will simply replace *q* by (n-1)/2 in our results. For a file of n = 2 particles, we can take advantage of the results obtained for the quadrant occupation time of the planar BM. Those results are recalled in section 1. Considering the particle of rank l = 2, i.e. the particle at the left end of the file, we immediately see that the four first moments $\langle u^k \rangle$ are known and given by equations (3)–(6). We deduce the corresponding moments for the rank l = 1 particle by using the equation (31).





Figure 4. For a file of n = 21 particles, computation of the moments $\langle u \rangle$ and $\langle u^2 \rangle$ as a function of the particle rank l $(1 \leq l \leq 21)$; (a) dots: equation (32), dashed line: the erfc function, equation (33); (b) dots: equation (36), dashed line: equation (40). We observe the agreement between the exact computation (dots) and the computation done in the limit of an infinite file of particles (dashed lines). The behaviours of $\langle u \rangle$ and $\langle u^2 \rangle$ look very similar. However, for l = 11, we have $\langle u \rangle = 1/2$ and $\langle u^2 \rangle = 0.339 \, 81... \approx 3/8 + (1/8) J_0(\pi) \approx 0.337$.

Table 2. The two first moments, $\langle u \rangle$ and $\langle u^2 \rangle$, for a particle of rank *l* belonging to a file of three particles.

l	$\langle u \rangle$	$\langle u^2 \rangle$
1	$\frac{7}{8}$	$\frac{1}{128} \left(105 - \frac{18}{\pi^2} \right) = 0.80606\dots$
2	$\frac{1}{2}$	$\frac{3}{8} - \frac{3}{16\pi^2} = 0.35600$
3	$\frac{1}{8}$	$\frac{1}{128} \left(9 - \frac{18}{\pi^2}\right) = 0.05606\dots$

4.2.1. The three particle case. For q = 1, equations (32) and (36) lead to the results quoted in table 2.

Looking at the values of $\langle u \rangle$ and $\langle u^2 \rangle$, we observe that the right-end (l = 1) particle spends most of its time on the x > 0 half-line. This is due to the middle particle (l = 2)that acts on it as a fluctuating and purely reflecting barrier [17]. The same argument holds for the left-end (l = 3) particle that spends most of its time on the x < 0 half-line. Let us now consider the middle (l = 2) particle. This one is subjected to the l = 1 and l = 3 particles that act as two fluctuating barriers that are typically located, respectively, in the x > 0 and x < 0 half spaces. As a consequence of the reflections, the middle particle is repelled towards the origin O, the U-shape distribution $P_2(u)$ is flattened and $\langle u^2 \rangle$ is decreased when compared to a single Brownian particle⁷.

⁷ In [17], the author shows that, for the middle particle, the diffusion constant D decreases when the number of particles in the file increases. However, we think that this decrease of D cannot be *directly* invoked to explain the decrease of $\langle u^2 \rangle$. Indeed, if we consider a single Brownian particle, its diffusion constant plays no role in the arc-sine law.





Figure 5. (a) The new integration domain—the interior of the pyramid $\underline{A'OC'B'D'}$. The saddle-point M_0 and the three perpendicular axes $\overline{M_0X'}, \overline{M_0Y'}, \overline{M_0Z'}$ are unchanged; h is the distance between the parallel lines (AB) and (A'B'); (b) the integration domain \mathcal{D}'' obtained by a translation of the domain \mathcal{D}' (displayed in figure 2(b)) along $\overline{M_0Y'}$.

$$\begin{array}{l}
4.2.2. The limit q \to \infty. \quad \text{To study this limit, we proceed as in section 3.3, equation (21):} \\
\sum_{m=0}^{2q+1-l} \sum_{k=0}^{2q+1-l-m} \sum_{r=0}^{2q+1-l-m} \frac{(2q+1)!(\pi+\phi)^{2q+1-k-r}(\pi-\phi)^{k+r}}{m!k!r!(2q+1-m-k-r)!} \\
\approx q^3 \int_{0}^{1-a'} \mathrm{d}X \int_{0}^{1-a'-X} \mathrm{d}Y \int_{0}^{1-a'-X} \mathrm{d}Z \exp(I(X,Y,Z))
\end{array}$$
(37)

where

$$a' = \frac{a}{\sqrt{q}} = \frac{l - (q+1)}{q}$$
; $-1 \leqslant a' \leqslant 1$

The new integration domain for X, Y, Z is shown in figure 5(a) and the saddle-point is unchanged.

Let us define h, the distance between the two parallel lines (AB) and (A'B'):

$$h = a'\sqrt{\frac{2}{3}} = \frac{a\sqrt{2}}{\sqrt{3q}}.$$

Still following the same lines as in section 3.3, we replace the integral I', equation (27), by:

$$I'' = \int_{\mathcal{D}''} dY' dZ' \exp\left(-q\left(\frac{3Y'^2}{2X_0} + \frac{Z'^2}{2(1-X_0)}\right)\right)$$
(38)

$$= 2 \int_{-\infty}^{-h} dY' \int_{0}^{(-h-Y')\sqrt{3}} dZ' \exp\left(-q\left(\frac{3Y'^2}{2X_0} + \frac{Z'^2}{2(1-X_0)}\right)\right)$$
(39)

The new integration domain \mathcal{D}'' , for Y' and Z', is displayed in figure 5(b): this is simply the domain \mathcal{D}' (see figure 2(b)) shifted by -h along the axis $\overline{M_0Y'}$.

Finally, after some algebra, we get:

$$\left\langle u^2 \right\rangle \equiv f(a) = \sqrt{\pi} \int_0^{1/2} \mathrm{d}x \frac{\sin(2\pi x)}{\sqrt{1-x}} \int_0^\infty \mathrm{d}y \, \mathrm{erf}\left(\frac{y}{\sqrt{x}}\right) \mathrm{e}^{-\frac{(y+a)^2}{(1-x)}} \tag{40}$$

where a has been defined in equation (35) and erf is the error function (see equation (34)).

Using the property equation (31), the result (33) and, also, observing that the change $l \to 2q+2-l$ only amounts to the change $a \to -a$, we get the relationship: $f(a) - f(-a) = -\operatorname{erf}(a)$. So, the odd part of f(a) is simply $-\frac{1}{2}\operatorname{erf}(a)$. Writing $f(a) = \sum_{0}^{\infty} c_n a^n$, we immediately deduce the odd coefficients

$$c_{2n+1} = \frac{(-1)^{n+1}}{\sqrt{\pi} \ n! \ (2n+1)} \tag{41}$$

Unfortunately, the situation is more tricky for the even coefficients. We only got the analytical results:

$$c_0 = \frac{3}{8} + \frac{1}{8}J_0(\pi) = 0.336\,96\dots \tag{42}$$

$$c_2 = \frac{\pi}{4} (H_0(\pi) - J_1(\pi)) = 0.18316...$$
(43)

 J_0 and J_1 are Bessel functions and H_0 is a Struve function [18] $(H_0(x) = \frac{2}{\pi} \int_0^{\pi/2} \sin(x \cos u) du).$

 $c_0 = f(0)$, equation (42), is simply the result (30) obtained for the middle particle in section 3.3.

In figure 4(b), we show the good agreement between the results (36) (for a file of n = 21 particles) and (40). We also observe that the distribution $P_l(u)$ is peaked at 0 (1) as soon as (l - (q + 1)) is of the order of $\sqrt{q} (-\sqrt{q})$.

5. Conclusion

In conclusion, we have studied analytically the occupation time T of the half-line [Ox) of a tracer particle among n hard-core Brownian particles starting all initially from O. These particles are labelled by their rank l and cannot cross each other. While the dynamics of the entire system is Markovian, the evolution of the only tracer is not, which makes this question a non-trivial problem. However, this problem can be mapped onto a single particle problem in \mathbb{R}^n , which allowed us to obtain explicit results for the two first moments of the occupation time T. Analytical results have been obtained for an arbitrary number n of Brownian particles and an arbitrary choice of the rank l of the tracer particle. The limit of an infinite number of particles $n \to \infty$ has been analyzed in detail.

Natural extensions of this work concern the case of arbitrary initial conditions and the determination of higher order moments. Another important generalization would be to reconsider the problem when the tracer particle is different from the other bath particles, and for example is the only particle to experience the effect of a bias.

References

- [1] Hahn K, Kärger J and Kukla V 1996 Phys. Rev. Lett. 76 2762
- [2] Wei Q-H, Bechinger C and Leiderer P 2000 Science 287 625
- [3] Meersmann T, Logan J W, Simonutti R, Caldarelli S, Comotti A, Sozzani P, Kaiser L G and Pines A 2000 J. Phys. Chem. A 104 11665
- [4] Lin B, Meron M, Cui B, Rice S A and Diamant H 2005 Phys. Rev. Lett. 94 216001
- [5] Harris T E 1965 J. Appl. Probab. 2 323
- [6] Rodenbeck C, Karger J and Hahn K 1998 Phys. Rev. E 57 04
- [7] Sanders L P, Lomholt M A, Lizana L, Fogelmark K, Metzler R and Ambjornsson T 2014 New J. Phys. 16 113050
- [8] Illien P, Bénichou O, Mejía-Monasterio, Oshanin G and Voituriez R 2013 Phys. Rev. Lett. 111 038102
- [9] Forsling R, Sanders L P, Ambjornsson T and Lizana L 2014 J. Chem. Phys. 141 094902
- [10] Levy P 1939 Compos. Math. 7 283
- [11] Levy P 1948 Processus Stochastiques et Mouvement Brownien (Paris: Editions Jacques Gabay)
- [12] Barlow M, Pitman J and Yor M 1989 Séminaire de Probabilités XXIII (Lecture Notes in Mathematics vol 1372) (Berlin: Springer) p 294
- [13] Desbois J 2002 J. Phys. A: Math. Gen. 35 L673
- [14] Bénichou O and Desbois J 2009 J. Phys. A: Math. Theor. 42 015004
- [15] Bingham N H and Doney R A 1988 J. Appl. Probab. 25 120
 Desbois J 2007 J. Phys. A: Math. Gen. 40 2251
- [16] Meyre T and Werner W 1995 Probab. Theory Relat. Fields 101 409
- [17] Aslangul Cl 1998 Europhys. Lett. 44 283
- [18] Gradstheyn I S and Ryzhik I M 1965 Table of Integrals, Series and Products (New York: Academic)