

## Velocity Anomaly of a Driven Tracer in a Confined Crowded Environment

Pierre Illien,<sup>1,\*</sup> Olivier Bénichou,<sup>1,†</sup> Gleb Oshanin,<sup>1</sup> and Raphaël Voituriez<sup>1,2</sup>

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

<sup>2</sup>Laboratoire Jean Perrin, FRE 3231 CNRS /UPMC, 4 Place Jussieu, 75255 Paris Cedex, France

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We consider a discrete model in which a tracer performs a random walk biased by an external force, in a dense bath of particles performing symmetric random walks constrained by hard-core interactions. We reveal the emergence of a striking velocity anomaly in confined geometries: in quasi-1D systems such as stripes or capillaries, the velocity of the tracer displays a long-lived plateau before ultimately dropping to a lower value. We develop an analytical solution that quantitatively accounts for this intriguing behavior. Our analysis suggests that such a velocity anomaly could be a generic feature of driven dynamics in quasi-1D crowded systems.

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In various physical and biological systems one encounters the situation when either an active particle or a particle subject to an external force travels through a quiescent host medium. A few stray examples include self-propelled particles in crowded environments, such as molecular motors, motile living cells or bacteria [1–3], or charge carriers biased by an external field [4,5]. Determining the dynamics of such a driven particle—called the tracer particle (TP) in what follows—in a host medium which hinders its motion is a challenging problem with important applications.

In particular, it constitutes a recurrent question of non-equilibrium statistical mechanics, arising in the quest of fundamental fluctuation-dissipation relations [6–8]. It is also the basis of the so-called active microrheology, which monitors the response of a medium while in the presence of a TP manipulated by an external force. Within recent years, this experimental technique has become a powerful tool for the analysis of such diverse systems as colloidal suspensions [9–13], glass forming liquids [14–18], fluid interfaces [19], or live cells [20,21]. A considerable amount of knowledge has been acquired on the forms of the so-called force-velocity relation  $v(F)$ —the dependence of the TP velocity  $v$  on the value of the applied force  $F$ .

The question of the behavior beyond the force-velocity relation was recently addressed in [15]. In this work, the dynamics of an externally driven TP in a glass-forming liquid was studied via molecular dynamics simulations. It was realized that although the TP is ultimately moving with a constant velocity  $v$  along the bias, (i.e.,  $\langle X_t \rangle \sim vt$ ), the variance  $\sigma_x^2 = \langle (X_t - \langle X_t \rangle)^2 \rangle$  of its position grows surprisingly in a superdiffusive manner,  $\sigma_x^2 \sim t^\lambda$ , with  $\lambda$  being within the range 1.3–1.5 (see also [16,18] for related studies).

A superdiffusive growth of the variance of the TP position along the bias has been established analytically

in a simple discrete model. In this model, the tracer performs a random walk biased by an external force, in a dense bath of particles performing symmetric random walks constrained by hard-core interactions [22–24]. In this model, the motion of the TP is mediated by successive visits of vacancies whose density is denoted  $\rho_0 = 1 - \rho$ , where  $\rho$  is the density of bath particles. It was found that in 2D and quasi-1D systems such as stripes or capillaries (see Fig. 1), there exists a long-lived superdiffusion induced by the anomalous return statistics of the vacancies to the TP position, crossing over to a diffusive behavior after a time  $t_x \approx 1/\rho_0^2$ . The complete time evolution of the variance was found to display a scaling behavior as a function of the scaled variable  $\rho_0^2 t$ , noted in Fig. 2 (inset) in the quasi-1D case.

Here, within the framework of the lattice gas model of [22–24], we show that in confined geometries not only the variance but already the *mean* of the TP displacement, (and, hence, the TP velocity  $v \sim \langle X_t \rangle / t$  itself), displays a striking anomaly, which has not apparently been noticed as of yet.

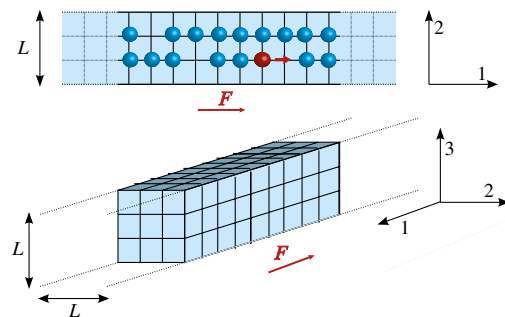


FIG. 1 (color online). A sketch of the confined geometries used in the numerical simulations and in the theoretical modeling (top: stripelike, bottom: capillarylike). Boundary conditions are periodic along directions 2 and 3. The TP, in red, is the only particle subject to the external force  $F$ .

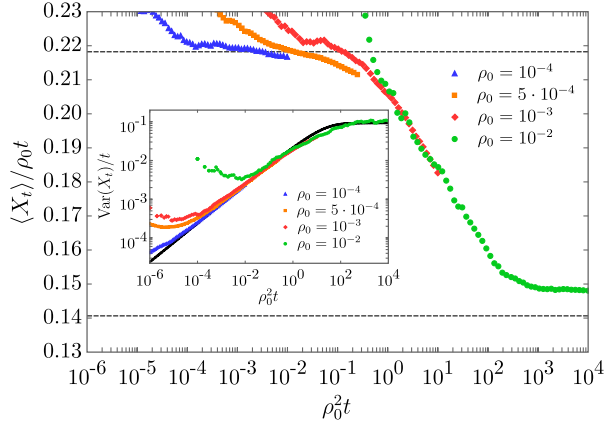


FIG. 2 (color online). Main plot: rescaled mean position of the TP as a function of rescaled time  $\rho_0^2 t$ , from numerical simulations in a 2D stripe with  $L = 3$  and an infinite external force. The dashed lines are the values of the velocity in the two limit regimes (see main text). Inset: rescaled variance as a function of rescaled time for the same system. The solid line is the analytical prediction from [24]. The number of realizations in numerical simulations ranges from  $10^2$  (for high  $\rho_0$ ) to  $10^5$  (for low  $\rho_0$ ).

We find that in dense systems the temporal evolution of the TP velocity consists of two distinct, clearly separated regimes: after a short transient  $v$  attains first a long-lived “high” constant value which persists up to times of order of  $t_x \sim 1/\rho_0^2$  and then rather abruptly drops to a terminal “low” constant value. This unexpected behavior, obtained from Monte Carlo numerical simulations in quasi-1D stripes, is plotted in Fig. 2 for several vacancy densities  $\rho_0$ , as a function of the rescaled variable  $\rho_0^2 t$ , as suggested by the scaling behavior of the variance. In this Letter we (i) calculate analytically the mean position of the TP in quasi-1D systems like stripes and capillaries in the dense limit  $\rho_0 \rightarrow 0$ , (ii) quantitatively account for the intriguing velocity anomaly reported above numerically, (iii) show that such an anomaly takes place beyond the linear response (in the linear response both velocities are equal), and (iv) show that it occurs only in quasi-1D systems, in contrast to superdiffusion which is observed in both quasi-1D and 2D systems, which implies that the velocity anomaly and the superdiffusive growth of the variance are not controlled by the same criteria.

*The model.*—We consider a quasi-1D system in dimension  $d \in \{2, 3\}$ , infinite in the direction 1, and finite with periodic boundary conditions in the other direction(s) (typically a two-dimensional stripe or a three-dimensional capillary; see Fig. 1). The lattice sites are occupied by hardcore particles, with density  $\rho$ , performing symmetric random walks, with the restriction that the occupancy number of each site is at most equal to 1 [25]. The vacancy density  $\rho_0 \equiv 1 - \rho$  is assumed to be very small (see [26] for a recent study in the opposite dilute limit  $\rho \ll 1$ ). The TP is initially placed at the origin and performs a random walk biased by an external force  $\mathbf{F} = F\mathbf{e}_1$ . In the usual fashion,

the TP jump probability in direction  $\nu$  is given by  $p_\nu = \exp(\frac{1}{2}\beta\sigma\mathbf{F} \cdot \mathbf{e}_\nu) / \sum_{\mu \in \{\pm 1, \dots, \pm d\}} \exp(\frac{1}{2}\beta\sigma\mathbf{F} \cdot \mathbf{e}_\mu)$ , where  $\beta$  is the inverse temperature and  $\sigma$  is the characteristic length of a single move.

More precisely the dynamics is as follows. At each time step  $t$ , each vacancy moves according to the following rules: (i) If the TP is not adjacent to the vacancy, one neighbor is randomly selected and exchanges its position with the vacancy; (ii) otherwise, if the TP is at position  $\mathbf{Y}$  and the vacancy at position  $\mathbf{Y} + \mathbf{e}_\nu$ , the TP exchanges its position with the vacancy with probability  $p_\nu / [(1 - 1/2d) + p_\nu]$  and with probability  $1/(2d - 1 + 2dp_\nu)$  with any of the  $2d - 1$  other neighbors; (iii) events involving two vacancies at the same site or on neighboring sites are of order  $\mathcal{O}(\rho_0^2)$  and do not contribute in the dense limit we consider here.

In the spirit of Refs. [27,28] where tracer diffusion in the absence of bias was studied, we first consider an auxiliary problem involving a single vacancy, starting from site  $\mathbf{Y}_0$ . The TP, initially at site  $\mathbf{0}$ , can move only by exchanging its position with the vacancy. For the sake of simplicity, we first present in detail the particular case where the applied force is strong enough for the TP motion to be directed, so that  $p_1 = 1$  and  $p_{\nu \neq 1} = 0$ . Results in the general case of arbitrary force, obtained along the same method, will be given next. The single-vacancy propagator  $P_t^{(1)}(\mathbf{X}|\mathbf{Y}_0)$  defined as the probability for the TP to be at site  $\mathbf{X} = \rho\mathbf{e}_1$  at time  $t$  can be written as

$$\begin{aligned}
 P_t^{(1)}(\mathbf{X}|\mathbf{Y}_0) &= \delta_{\rho,0} \left( 1 - \sum_{j=0}^t F_j^*(\mathbf{Y}_0) \right) \\
 &+ \sum_{m_1=1}^{+\infty} \dots \sum_{m_p=1}^{+\infty} \sum_{m_{p+1}=0}^{+\infty} \delta_{m_1+\dots+m_{p+1},t} \\
 &\times \left( 1 - \sum_{j=0}^{m_{p+1}} F_j^*(-\mathbf{e}_1) \right) F_{m_p}^*(-\mathbf{e}_1) \times \dots \times \\
 &F_{m_2}^*(-\mathbf{e}_1) F_{m_1}^*(\mathbf{Y}_0), \quad (1)
 \end{aligned}$$

where  $F_t^*(\mathbf{Y}_0)$  is the probability that the vacancy, which starts its random walk at the site  $\mathbf{Y}_0$ , arrives at the origin  $\mathbf{0}$  for the first time at the time step  $t$ , and where the second sum in Eq. (1) is equal to zero if  $p \leq 0$ . The first term in the right-hand side of Eq. (1) represents the event that at time  $t$ , the TP has not been visited by the vacancy, while the second one results from a partition on the waiting times  $m_j$  between the successive visits of the TP by the vacancy. The Fourier-Laplace transform of the single-vacancy propagator is then easily found to be given by

$$\hat{P}^{(1)}(\mathbf{k}|\mathbf{Y}_0; \xi) = \frac{1}{1 - \xi} \left[ 1 + \frac{\hat{F}^*(\mathbf{Y}_0; \xi)(e^{ik_1} - 1)}{1 - e^{ik_1} \hat{F}^*(\mathbf{e}_{-1}; \xi)} \right], \quad (2)$$

where the discrete Laplace transform of a time-dependent function  $\phi(t)$  has been denoted by  $\hat{\phi}(\xi) = \sum_{t=0}^{\infty} \phi(t)\xi^t$  and the Fourier transform of a space-dependent function  $\psi(\mathbf{r})$  by  $\tilde{\psi}(\mathbf{k}) = \sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}}\psi(\mathbf{r})$ .

The second step of the calculation consists of reducing in the dense limit  $\rho_0 \rightarrow 0$  the full problem to the single-vacancy problem. This is conveniently done by starting from a finite number  $M$  of vacancies, of initial positions  $\mathbf{Y}_0^{(1)}, \dots, \mathbf{Y}_0^{(M)}$  on a finite lattice of  $N$  sites. The key point is that, in the limit  $\rho_0 = M/N \rightarrow 0$ , the vacancies contribute independently to the motion of the TP [28], so that the full propagator can be written to leading order in  $\rho_0$  in terms of the single vacancy propagator,

$$P_t(\mathbf{X}|\mathbf{Y}_0^{(1)}, \dots, \mathbf{Y}_0^{(M)}) \underset{\rho_0 \rightarrow 0}{\sim} \sum_{\mathbf{X}_0^{(1)}} \dots \sum_{\mathbf{X}_0^{(M)}} \delta_{\mathbf{x}, \mathbf{X}_0^{(1)} + \dots + \mathbf{X}_0^{(M)}} \times \prod_{j=1}^M P_t^{(1)}(\mathbf{X}_0^{(j)}|\mathbf{Y}_0^{(j)}). \quad (3)$$

Averaging next over the initial positions of the vacancies, taking the Fourier transform and finally going to the thermodynamic limit, the logarithm of the Fourier transform of the propagator can be written to leading order in  $\rho_0$  as  $\ln \tilde{P}_t(\mathbf{k}) \underset{\rho_0 \rightarrow 0}{\sim} -\rho_0 \hat{\Omega}_t(\mathbf{k})$ , where

$$\hat{\Omega}(\mathbf{k}; \xi) = \left[ \frac{1}{1-\xi} - e^{i\mathbf{k}_1} \hat{P}^{(1)}(\mathbf{k}|\mathbf{e}_{-1}; \xi) \right] \sum_{\mathbf{Y} \neq \mathbf{0}} \hat{F}^*(\mathbf{Y}; \xi). \quad (4)$$

Noting that the mean position of the TP in the direction of the bias is given by

$$\langle X \rangle(\xi) \underset{\rho_0 \rightarrow 0}{\sim} i\rho_0 \left. \frac{\partial \hat{\Omega}}{\partial k_1} \right|_{\mathbf{k}=\mathbf{0}}, \quad (5)$$

it is finally found to leading order in  $\rho_0$  that

$$\langle X \rangle(\xi) \underset{\rho_0 \rightarrow 0}{\sim} \frac{\rho_0 \sum_{\mathbf{Y} \neq \mathbf{0}} \hat{F}^*(\mathbf{Y}; \xi)}{(1-\xi)[1 - \hat{F}^*(\mathbf{e}_{-1}; \xi)]}. \quad (6)$$

The last step of the calculation consists of determining the large time behavior of the first-passage time densities  $F^*$ , or, equivalently, the behavior  $\xi \rightarrow 1$  of their discrete Laplace transform  $\hat{F}^*$  involved in Eq. (6). Since the vacancy performs a symmetric random walk except in the very vicinity of the TP site, it is conveniently done by applying standard methods of random walks with defective sites described in [29], the defective sites being here the site occupied by the TP and its nearest neighbors. Lengthy but standard calculations yield in the limit  $\xi \rightarrow 1$  (associated to the large time limit)

$$\hat{F}^*(\mathbf{e}_{-1}; \xi) = 1 - \frac{1}{a_0 G(\xi)} + \mathcal{O}(1-\xi), \quad (7)$$

TABLE I. Explicit expressions of  $G(\xi)$  and  $\alpha$  for 2D and quasi-1D systems.

Lattice	$G(\xi)$	$\alpha$
2D infinite	$(1/\pi) \ln[1/(1-\xi)]$	$4 - (8/\pi)$
2D stripe	$1/(L\sqrt{1-\xi})$	$8 - 8S_{L,1}^{(2)} - 8S_{L,3}^{(2)}$
3D capillary	$\sqrt{6}/(2L^2\sqrt{1-\xi})$	$18 - 16S_{L,0}^{(3)} + 12S_{L,1}^{(3)} - 2S_{L,2}^{(3)}$

$$\sum_{\mathbf{Y} \neq \mathbf{0}} \hat{F}^*(\mathbf{Y}; \xi) = \frac{1}{(1-\xi)G(\xi)} + \mathcal{O}(1), \quad (8)$$

where  $G(\xi)$  is the leading order term of  $\hat{P}(\mathbf{0}|\mathbf{0}; \xi)$  when  $\xi \rightarrow 1$  and  $\hat{P}(\mathbf{r}|\mathbf{r}_0; \xi)$  is the discrete Laplace transform of the propagator of a usual nearest-neighbor symmetric random walk and

$$a_0 \equiv \frac{2d - \alpha}{2d + (2d - 1)\alpha}, \quad (9)$$

$$\alpha \equiv \lim_{\xi \rightarrow 1^-} [\hat{P}(\mathbf{0}|\mathbf{0}; \xi) - \hat{P}(2\mathbf{e}_1|\mathbf{0}; \xi)]. \quad (10)$$

Explicit expressions of  $G(\xi)$  and  $\alpha$  for 2D and quasi-1D systems are provided in Table I, where we defined

$$S_{L,n}^{(2)} = \frac{1}{L} \sum_{k=1}^{L-1} \frac{\sin^n(\pi k/L)}{\sqrt{1 + \sin^2(\pi k/L)}}, \quad (11)$$

$$S_{L,n}^{(3)} = \frac{1}{L^2} \sum_{\substack{k_2, k_3=0 \\ (k_2, k_3) \neq (0,0)}}^{L-1} [\cos(2\pi k_2/L) + \cos(2\pi k_3/L)]^n \times \left[ \left( 1 + \frac{1}{3} [\cos(2\pi k_2/L) + \cos(2\pi k_3/L)] \right)^2 - \frac{1}{9} \right]^{-1/2}. \quad (12)$$

Finally, we have that  $\langle X \rangle(\xi) \sim \rho_0 a_0 / (1-\xi)^2$ , and, hence, using a Tauberian theorem, we get

$$\lim_{\rho_0 \rightarrow 0} \frac{\langle X_t \rangle}{\rho_0} \underset{t \rightarrow \infty}{\sim} a_0 t. \quad (13)$$

This calculation can be extended to the case of arbitrary jump probabilities  $p_\nu$  of the TP and Eq. (13) is found to hold in this general case with

$$a_0 \equiv \frac{p_1 - p_{-1}}{1 + \frac{2d\alpha}{2d-\alpha}(p_1 + p_{-1})}. \quad (14)$$

This explicit expression provides a value of the velocity which is in good quantitative agreement with the high

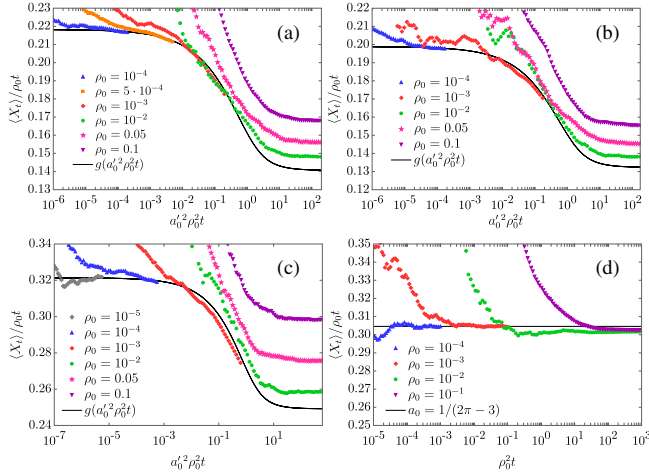


FIG. 3 (color online). Rescaled mean position of the TP as a function of rescaled time, for different geometries and forces. (a) 2D stripe with  $L = 3$  and infinite external force. (b) 2D stripe with  $L = 3$  and  $F = 4$ ,  $\beta\sigma = 1$ . (c) 3D capillary with  $L = 3$  and infinite external force. For (a),(b), and (c), the solid line is the scaling function  $g$  defined in the main text. (d) 2D infinite lattice with infinite drag force. The solid line is the single value  $a_0 = a_0'$ . The number of realizations in numerical simulations ranges from  $10^2$  (for high  $\rho_0$ ) to  $10^5$  (for low  $\rho_0$ ).

velocity obtained numerically at short times (see Fig 2 for  $p_1 = 1$  and Fig 3 for  $p_1 < 1$ ).

In order to describe the ultimate regime corresponding to the low velocity we now need to analyze the regime where the large time limit is taken first and the small density limit next [in contrast to the regime considered in Eq. (13)]. The formalism described above can actually be extended to analyze this second limit. The key difference with the previous case is that for a *fixed* small  $\rho_0$  the random walk performed by the vacancy between two successive visits of the lattice site occupied by the TP is a *biased* random walk in the reference frame of the TP, due to the interactions of the TP with the other vacancies. The method presented above can then be applied, provided that the symmetric propagators  $\hat{P}$  are replaced by biased propagators  $\hat{P}^\epsilon$  (that can be explicitly evaluated). In the dense limit  $\rho_0 \rightarrow 0$ , the bias  $\epsilon$  is proportional to the vacancy density  $\rho_0$  so that its explicit determination is not needed to determine the velocity to leading order. It is finally found that

$$\lim_{t \rightarrow \infty} \frac{\langle X_t \rangle}{t} \Big|_{\rho_0 \rightarrow 0} \sim \rho_0 a_0',$$

$$\frac{1}{a_0'} \equiv \frac{1}{a_0} + \frac{4d^2}{(2d - \alpha)L^{d-1}}, \quad (15)$$

where  $\alpha$  is still defined by Eq. (10) with unbiased propagators. Several comments are in order. (i) In quasi-1D systems, the transverse width  $L$  is finite, so that the ultimate velocity  $\rho_0 a_0'$  is always lower than the first high velocity  $\rho_0 a_0$ . The theoretical expressions Eqs. (13), (15)

quantitatively account for the velocity anomaly numerically evidenced in Fig. 2 [see also Figs. 3(a), 3(b), and 3(c)]; note that the theoretical low value is reached only in the limit  $\rho_0 \rightarrow 0$ , which explains the observed discrepancy between the theoretical and numerical values that decreases when  $\rho_0 \rightarrow 0$ . (ii) The velocity jump  $\rho_0(a_0 - a_0')$  can be shown to scale as  $F^2$  for small applied force  $F$ , so that this anomaly emerges beyond the linear response. In turn, to linear order in  $F$ , there is a single velocity which can be shown to fulfill the Einstein relation; (iii) this velocity jump can be checked to be a decreasing function of  $L$ , in systems unbounded in the transverse direction, i.e., such that  $L \rightarrow \infty$ ,  $a_0' = a_0$  which means that no velocity anomaly occurs. In particular, in infinite 2D systems, superdiffusion takes place but no velocity anomaly is observed, as numerically confirmed in Fig. 3(d) (note that this single value of the velocity had already been obtained in [30]); (iv) mathematically, the criteria for superdiffusion to occur is that the limits  $\epsilon \rightarrow 0$  and  $\xi \rightarrow 1$  of  $\widehat{P}^\epsilon(\mathbf{0}|\mathbf{0}; \xi)$  do not commute [24], which is the case in 2D and quasi-1D systems. The condition for velocity anomaly is in contrast to the fact that the limits  $\epsilon \rightarrow 0$  and  $\xi \rightarrow 1$  of  $\widehat{P}^\epsilon(\mathbf{0}|\mathbf{0}; \xi) - \widehat{P}^\epsilon(2\mathbf{e}_1|\mathbf{0}; \xi)$  do not commute, which is in fact more constraining, and is satisfied in quasi-1D systems but not in 2D systems. Parenthetically, we note that this noncommutation of the limits for  $\widehat{P}^\epsilon(\mathbf{0}|\mathbf{0}; \xi) - \widehat{P}^\epsilon(2\mathbf{e}_1|\mathbf{0}; \xi)$  is a general property which holds for any biased random walk in quasi-1D systems, and could potentially have implications in other contexts.

Therefore, in quasi-1D systems, two different regimes of the velocity have been identified. In fact, the complete dynamics of the mean position of the TP can be obtained in the scaling regime  $t \rightarrow \infty$  and  $\rho_0 \rightarrow 0$  with  $\rho_0^2 t$  fixed. We find that in this limit

$$\frac{\langle X_t \rangle}{\rho_0 t} \sim g(a_0'^2 \rho_0^2 t), \quad (16)$$

with

$$g(\tau) = a_0 \left\{ \frac{b}{b^2 - 1} \left[ \operatorname{erf}(\sqrt{\tau}) + \frac{e^{-\tau}}{\sqrt{\pi\tau}} \right] + \frac{1}{\tau} \left( \frac{b}{b^2 - 1} \right)^2 \left[ e^{(b^2-1)\tau} [1 - \operatorname{erfc}(b\sqrt{\tau})] - 1 \right] + \frac{b}{2} \frac{b^2 + 1}{(b^2 - 1)^2} \frac{\operatorname{erf}(\sqrt{\tau})}{\tau} - \frac{1}{b^2 - 1} \right\}, \quad (17)$$

where  $b \equiv a_0/a_0' - 1$ . Note that this scaling function reproduces both regimes (13) and (15) by taking the appropriate limits. Figures 3(a), 3(b), and 3(c) show a very good agreement for all time scales with numerical simulations for 2D stripes and 3D capillaries.

In conclusion, on the basis of a simple model of a driven diffusive tracer in a crowded environment, our analysis has



revealed the emergence of a striking velocity anomaly in confined geometries. Namely, we have shown that in quasi-1D systems such as stripes or capillaries, which are used nowadays in nanofluidics [31], the TP velocity, which is a prominent observable of microrheology, displays a long-lived plateau before ultimately dropping to a lower value. We have developed an analytical solution that quantitatively accounts for this intriguing behavior. Physically, the high value of the velocity originates from repeated interactions of the TP with a single vacancy that performs a recurrent random walk in low dimensions. After a time scale  $t_x \approx 1/\rho_0^2$ , other vacancies start interacting with the TP, and lead ultimately to the emergence of the low velocity. A subtle point, quantified by the expressions (13) and (15) is that this velocity jump is actually strictly equal to zero in infinite 2D systems. In particular, velocity anomaly occurs only in quasi-1D systems in contrast to superdiffusive growth of the variance of the TP position which is observed in both quasi-1D and 2D systems. Finally, our analysis suggests that velocity anomaly could be a generic feature of driven dynamics in quasi-1D crowded systems.

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\*illien@lptmc.jussieu.fr

†benichou@lptmc.jussieu.fr

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