Tagged particle diffusion in single file systems

Henk van Beijeren

Institute for Theoretical Physics
Utrecht University

Universiteit Utrecht

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Most interest goes to the dynamics of tagged particles moving within a single file.

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Warning! For clearly seeing interesting behavior one has to use this identity by preference in a coordinate frame where the tagged particle on average has no drift. In general one has

$$< (x_j(t) - x_j(0))^2 > \approx (vt)^2 + \frac{1}{n^2} < \left(\int_0^t d\tau\, j(0,\tau) \right)^2 >_{mf}$$

but the integrated current in the rest frame exhibits additional fluctuations, which may be larger than the second term.

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$$\int_0^t d\tau\,\widehat{j}(k,\tau) = -\frac{\widehat{n}(k,t)-\widehat{n}(k,0)}{ik} \qquad (k \neq 0)$$

$$k = 0 \rightarrow \qquad \int_0^t d\tau\,\widehat{j}(0,\tau) = N\big(X(t)-X(0)\big)$$

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$$<\left(x_j(t)-x_j(0)\right)^2> = \frac{1}{(nL)^2}\sum_{k\neq 0}\frac{<\left(\widehat{n}(k,t)-\widehat{n}(k,0)\right)\left(\widehat{n}(-k,t)-\widehat{n}(-k,0)\right)>}{k^2}$$

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$$+\frac{N^2<\left(X(t)-X(0)\right)^2>}{(nL)^2}$$

$$=\sum_{k\neq 0}\frac{2S(k)-\left(S(k,t)+S(-k,t)\right)}{Nnk^2}+<\left(X(t)-X(0)\right)^2>$$

with

$$S(k,t)=\frac{<\hat{n}(k,t)\hat{n}(-k,0)>}{L}$$

$$< \left(x_j(t) - x_j(0) \right)^2 >= \frac{1}{(nL)^2} \sum_{k \neq 0} \frac{< \left(\widehat{n}(k,t) - \widehat{n}(k,0) \right) \left(\widehat{n}(-k,t) - \widehat{n}(-k,0) \right) >}{k^2}$$

$$+ \frac{N^2 < \left(X(t) - X(0) \right)^2 >}{(nL)^2}$$

$$= \sum_{k \neq 0} \frac{2S(k) - \left(S(k,t) + S(-k,t) \right)}{Nnk^2} + < \left(X(t) - X(0) \right)^2 >$$

with

$$S(k,t) = \frac{< \widehat{n}(k,t) \widehat{n}(-k,0) >}{L}$$

in limit $L \to \infty$

$$< \left(x_j(t) - x_j(0)^2 \right) >= \frac{1}{2\pi} \int dk \frac{2S(k) - \left(S(k,t) + S(-k,t) \right)}{(nk)^2} + \left(Vt \right)^2$$

Applications

The simplest cases are those were particles move independently but exchange identities on passing each other (equivalent to asking: “what is the displacement of the 138th particle in the queue?”).

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In that case: $S(k,t) = nS_{single}(k,t)$ with $S_{single}(k,t) =< e^{-ik(x(t)-x(0))} >$

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Suppose: $S(k,t) = S(k)\, f(kt^{1/\alpha})$

$$\Rightarrow \qquad < \left(x_{free}(t) - x_{free}(0) \right)^2 > \; = \; -\left(\frac{\partial^2 S(k,t)}{\partial k^2} \right)_{k=0} \sim t^{2/\alpha}$$

but $< \left(x_j(t) - x_j(0) \right)_{sf}^2 > \; \sim t^{1/\alpha}$ provided V=0!

Known as Percus’ rule

The simplest cases are those were particles move independently but exchange identities on passing each other (equivalent to asking: "what is the displacement of the 138th particle in the queue?").

Examples:

1) Jepsen gas. Point particles of equal mass move ballistically and exchange velocities on colliding.

$$S(k,t) = \left\langle \frac{1}{L} \sum_{jl} e^{ik\left(x_j(0) - x_l(t)\right)} \right\rangle = \frac{1}{L} \left\langle \sum_j e^{-ikv_j t} \right\rangle = n \int dv \;\varphi(v)\; e^{-ikvt}$$

$$\Rightarrow \qquad \left\langle \left(x_j(t) - x_j(0)\right)^2_{sf} \right\rangle = \frac{\langle |v| t \rangle}{n}$$

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Non-crossing Brownian particles (T.E. Harris)

In this case:

$$< \left(x_j(t) - x_j(0) \right)^2_{sf} > \; = \frac{1}{\pi n} \int dk \; \frac{1 - e^{-Dk^2 t}}{k^2} = \frac{2}{n} \sqrt{\frac{Dt}{\pi}}$$

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For Brownian particles with drift, add $(Vt)^2$.

Lévy flights: random flights with power law jump length distribution,

$$S(k,t) = n e^{-\mathcal{D}|k|^{\alpha} t}$$

For these one finds:

$$< \left(x_j(t) - x_j(0) \right)^2_{sf} > \; = \frac{1}{\pi n} \int dk \; \frac{1 - e^{-\mathcal{D}|k|^{\alpha} t}}{k^2} = \Gamma\left(\frac{\alpha - 1}{\alpha} \right) \left(\mathcal{D} t \right)^{1/\alpha}$$

requires $\alpha > 1$ for convergence

For long times the distribution of the displacement of the tagged particle in AP approximation becomes Gaussian, thanks to the central limt theorem. The roughly $N/2$ particles that are initially to the right of the origin are identically distributed and have the same probability of having passed the origin at time t. So the distribution for the number having passed the origin becomes approximately gaussian for large enough times. This then also holds for the difference of numbers passing in either direction.

This in principle will work for any type of independent particle dynamics with uniform stationary density.

Second category: Interacting systems

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Collective dynamics is diffusive, so same results as for independent Brownian particles.

ASEP. Same but with asymmetric hopping rates. In this model the average drift velocity of a tagged particle always differs from the velocity at which perturbations of the density move through the system. Hence, fluctuations in the integrated mass flow through the origin typically grow as the square root of its average, that is ~ $t^{1/2}$.

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Could it be possible getting a tagged particle speed equal to the pattern velocity?

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Could it be possible getting a tagged particle speed equal to the pattern velocity?

Should be doable by adding additional species, e.g. second class particles with suitable jump rates. For this case one expects a MSD $\sim t^{2/3}$ corresponding to KPZ behavior of the collective structure function, $S(k,t)=f(k\, t^{2/3})$.

Hamiltonian dynamics.

For 1d single component Hamiltonian systems with short ranged interactions the structure function exhibits two sound peaks (Brillouin peaks) and one, central heat peak (Rayleigh peak).

Their behavior is expected to be governed by the 1-dimensional KPZ equation, leading to

$$S(k,t) = \sum_{\sigma=\pm} S^{\sigma}(k,t) + S^{H}(k,t)$$

$$S^{\sigma}(k,t) = e^{-i\sigma ckt} f_{KPZ}(Ckt^{2/3})$$

$$S^{H}(k,t) = e^{-\alpha k^{5/3} t}$$ like for Lévy flights

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$$S^{H}(k,t) = e^{-\alpha k^{5/3} t}$$

Gives rise to three contributions to MSD:

$$\mathrm{S}^{\sigma} \Rightarrow \; ct$$

$$\mathrm{S}^{H} \Rightarrow \; t^{3/5}$$

Finite size effects

Consider first Hamiltonian systems with fixed center of mass and periodic boundary conditions.

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Due to the fixation of the CM the k=0 term in the AP summation form vanishes. So one misses $<V^2_{CM}>t^2$.

The fixed center of mass also constrains the displacement of a tagged particle to $L(N\text{-}1)/N$. So the MSD saturates for long times. In the limit $t \longrightarrow \infty$ one obtains

$$< \left(x_j(t) - x_j(0) \right)^2 > = < \left(x_j(t) - < x_j > - (x_j(0) - < x_j >) \right)^2 >$$

$$= 2 < \left(x_j - < x_j > \right)^2 >$$

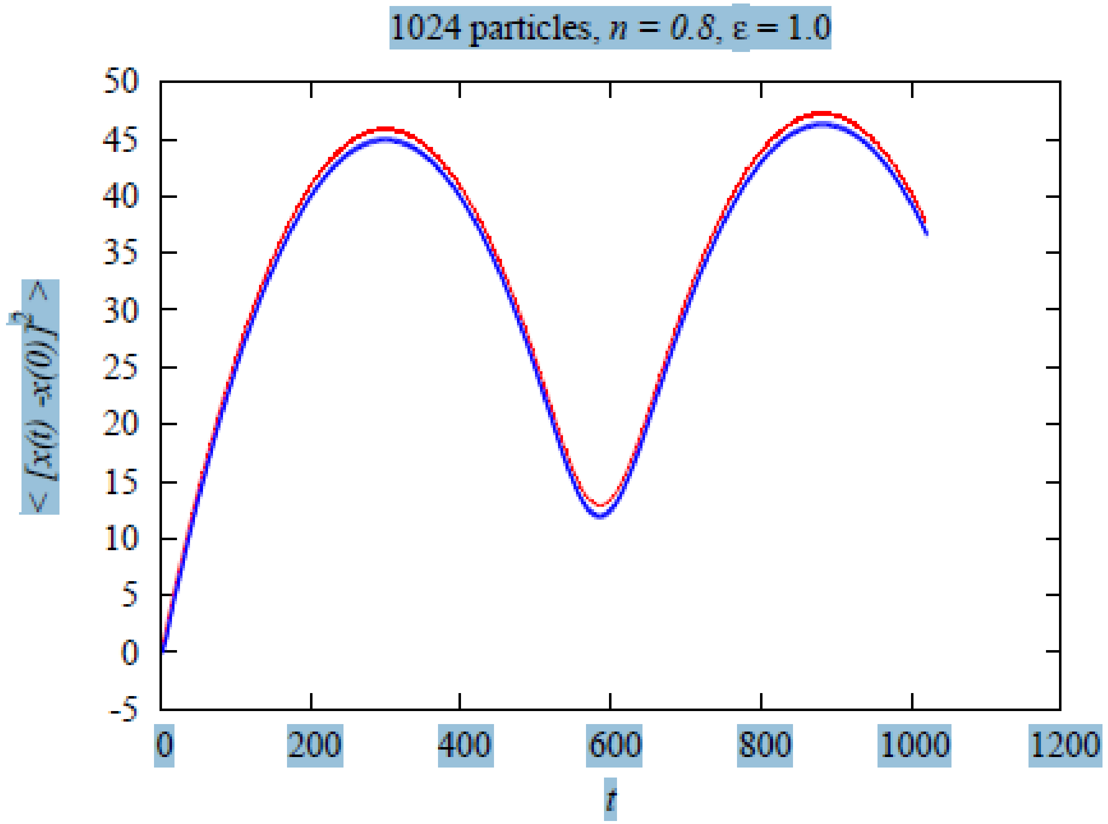

FIG. 2: Comparison of mean-squared deviation (MSD) (with error bars) for $N = 1024$.

Red: simulation value;
blue: Alexander-Pincus approximation
based on simulation values for S(k,t)

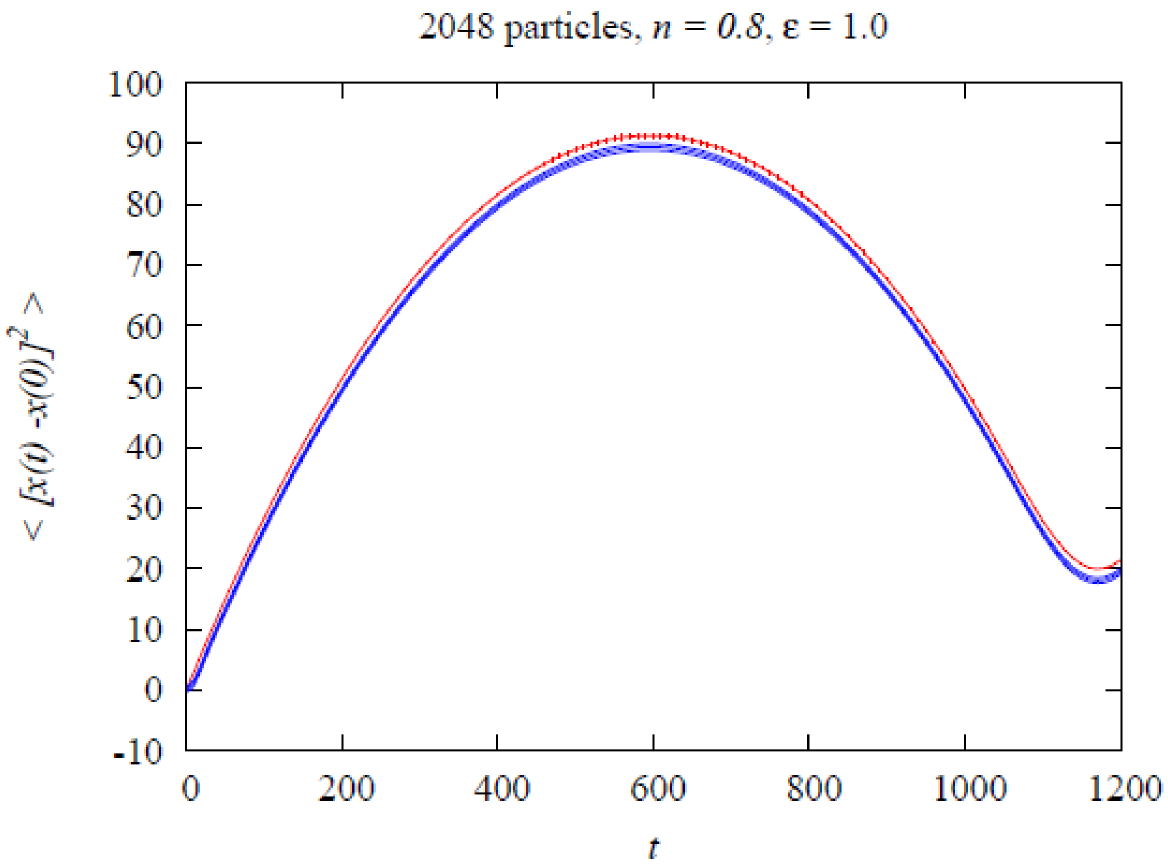

FIG. 3: Comparison of mean-squared deviation MSD (with error bars) for $N = 2048$.

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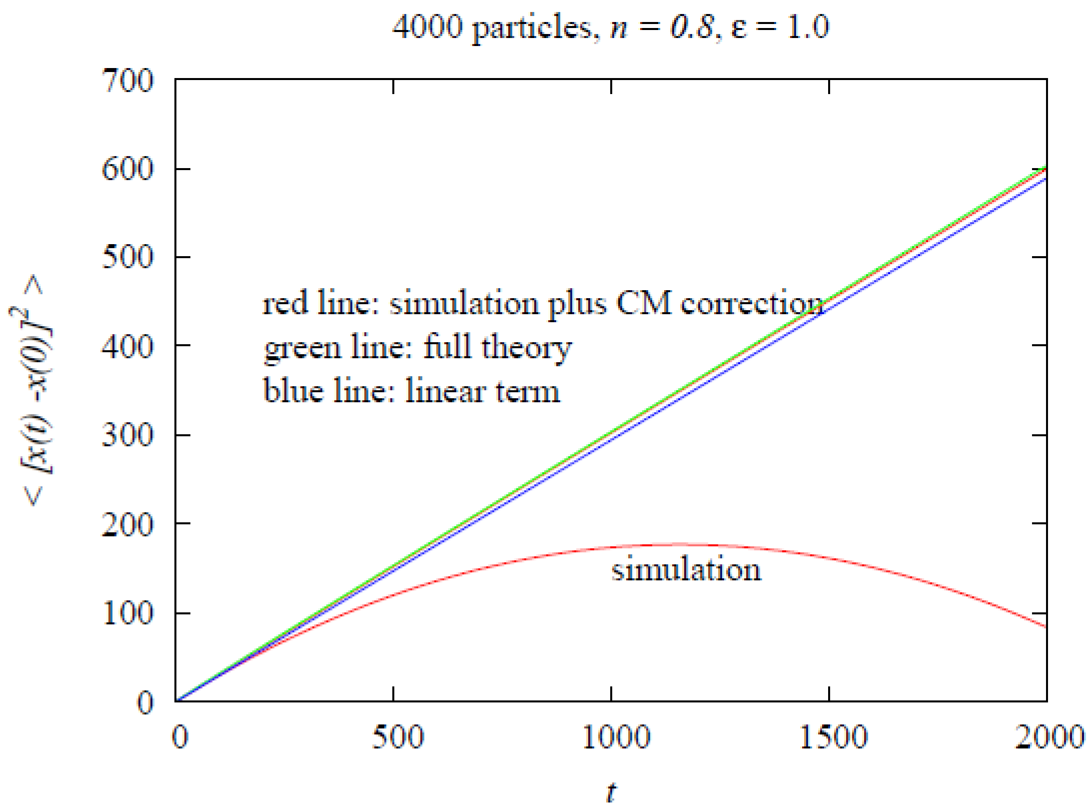

FIG. 7: Comparison of experimental and theoretical MSD for 4000 particles.

Finite size effects in diffusive systems with PBC

For long times CM performs diffusive motion with $D_{CM}=D/N$.

For a tagged particle:

$$
\begin{aligned}
< \left(x_j(t) - x_j(0) \right)^2 > = & < ((x_j(t) - < x_j(t) >_{X(t)}) - (x_j(0) - < x_j(0) >_{X(0)}) \\
& + (< x_j(t) >_{X(t)} - < x_j(0) >_{X(0)}))^2 > \\
= & < \left(X(t) - X(0) \right)^2 > + 2 < \left(x_j - < x_j >) \right)^2 >_X
\end{aligned}
$$

So for large t this differs from the Hamiltonian result only by an additional amount $2Dt/N$.

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