Dynamics and Correlations of a Tracer in a Linear Chain of Run-and-Tumble Particles

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ICTS

A few models to mimic active particles:

$$\dot{\mathbf{r}}_i = -\mu \nabla_i \Phi + \mathbf{v}_i$$

(a) Run-and-tumble particle

$$v_i = v_0 \sigma_i, \qquad \sigma_i = +1, -1$$

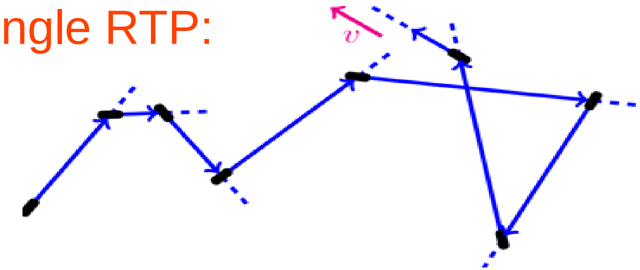
(b) Active Brownian particle

$$v_i = f_p \hat{\theta}_i, \qquad \frac{d\theta_i}{dt} = \sqrt{(2D_{rot})}\,\eta_i$$

(c) Active Ornstein-Uhlenbeck particle

$$\tau \dot{v}_i = -v_i + \sqrt{(2D)}\,\eta_i$$

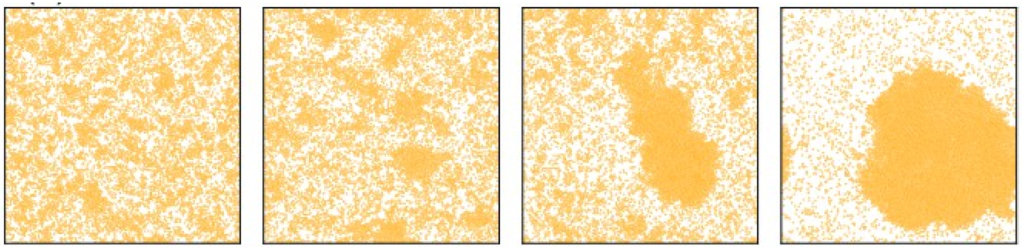
Single RTP:



$$\langle \Delta x^2 \rangle_{\mathrm{RTP}} = \left(\frac{v_{\mathrm{R}}}{\gamma}\right)^2 \left(\gamma t - \frac{1 - e^{-2\gamma t}}{2}\right) + 2Dt,$$

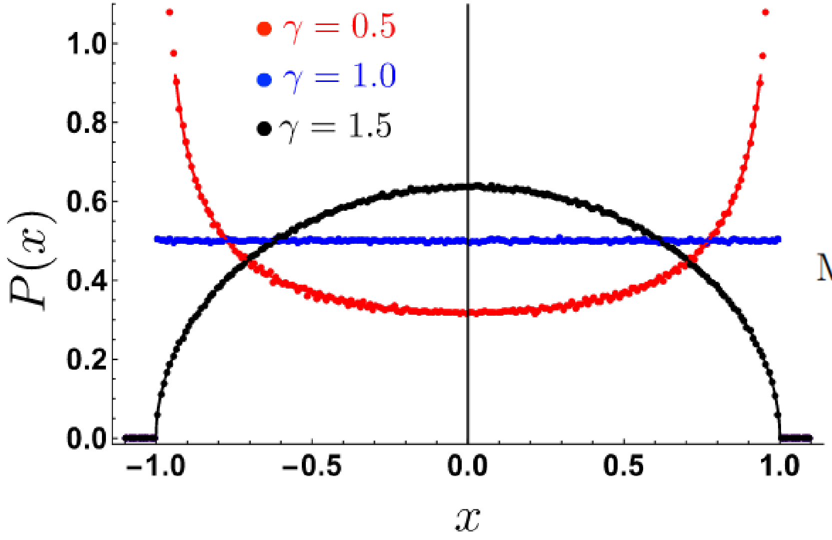
$$\langle \Delta x^2 \rangle_{\mathrm{ABP}} = \left(\frac{v_{\mathrm{A}}}{D_{\mathrm{r}}}\right)^2 \left(D_{\mathrm{r}} t - 1 + e^{-D_{\mathrm{r}} t}\right) + 2Dt,$$

$$\langle \Delta x^2 \rangle_{\mathrm{AOUP}} = 2(v_{\mathrm{O}}\tau)^2 \left(\frac{t}{\tau} - 1 + e^{-t/\tau}\right) + 2Dt.$$



MIPS with ABP

Single RTP in a harmonic potential:



$$V(x) = \frac{1}{2} k x^2$$

$$\frac{dx}{dt} = -kx + v_0 \sigma(t)$$

$$\mathrm{MSD} = \langle [x(t) - x(0)]^2 \rangle = \frac{2v_0^2}{k(k+2\gamma)} - \frac{2v_0^2}{(2\gamma+k)} \left[\frac{e^{-kt}}{k} + \frac{e^{-2\gamma t} - e^{-kt}}{k - 2\gamma} \right].$$

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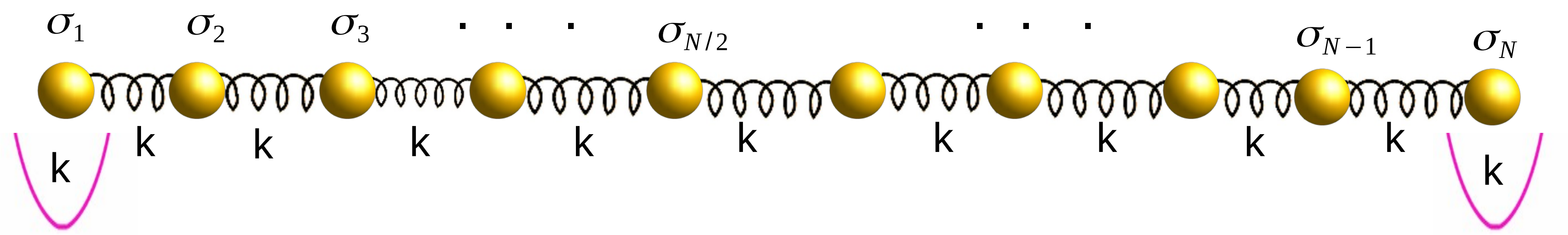
Model and observables:



$$\dot{x}_l = -k(2x_l - x_{l-1} - x_{l+1}) + v_0\sigma_l \qquad \langle \sigma_l(t_1)\sigma_m(t_2)\rangle = e^{-2\alpha|t_1-t_2|}\delta_{l,m}$$

Mean-squared displacement:

$$\Delta_l(t) = \lim_{t_0\to\infty} \langle [x_l(t+t_0) - x_l(t_0)]^2 \rangle$$

Displacement distribution of the bulk tracer:

$$P(\delta x_{N/2}, t)$$

Two-point correlations:

$$C^x_{l,m}(t) = \lim_{t_0\to\infty} \left[\langle x_l(t_0)x_m(t_0+t)\rangle - \langle x_l(t_0)\rangle\langle x_m(t_0+t)\rangle\right].$$

$$C^y_{l,m}(t) = \lim_{t_0\to\infty} \left[\langle y_l(t_0)y_m(t_0+t)\rangle - \langle y_l(t_0)\rangle\langle y_m(t_0+t)\rangle\right].$$ with $y_l(t) = x_{l+1}(t) - x_l(t)$

Equations of motion and definitions:

$$\dot{X} = -\Phi X + v_0 \Sigma \xrightarrow[\text{Transform}]{\text{Fourier}} \tilde{X}(\omega) = v_0 \tilde{\mathcal{G}}(\omega)\ \tilde{\Sigma}(\omega)\,,$$

with,

where, $\tilde{\mathcal{G}}(\omega) = (i\omega \mathbb{1} + \Phi)^{-1}$, $\quad \Phi_{l,m} = k(2\delta_{l,m} - \delta_{l,m-1} - \delta_{l,m+1})\,,$

$$\begin{aligned} C^x(t) &= \langle X(t) X^T(0) \rangle \\ &= \frac{v_0^2}{4\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{\mathcal{G}}(\omega_1) \left\langle \tilde{\Sigma}(\omega_1) \tilde{\Sigma}^T(\omega_2) \right\rangle \tilde{\mathcal{G}}^T(\omega_2) e^{i\omega_1 t}\ d\omega_1\ d\omega_2 \end{aligned}$$

$$\begin{aligned} C^x_{l,m}(t) &= 2v_0^2 \alpha \sum_{s=1}^{N} \frac{\phi_s(l)\phi_s(m)}{4\alpha^2 - \lambda_s^2} \left(\frac{e^{-\lambda_s t}}{\lambda_s} - \frac{e^{-2\alpha t}}{2\alpha} \right) \\ &= \frac{2v_0^2 \alpha}{\pi} \int_{-\infty}^{\infty} d\omega \frac{e^{i\omega t}}{4\alpha^2 + \omega^2} F_{l,m}(\omega) \end{aligned}$$

where $\phi_s(i) = \langle i | s \rangle.$

where $F_{l,m}(\omega) = -\frac{1}{\omega} \mathrm{Im} \left[\frac{\sin(lq)\sin(N-m+1)q}{\sin(q)\sin((N+1)q))} \right]$ for $l \leq m$

In Fourier space:

$$\langle \tilde{\sigma}(\omega_1) \tilde{\sigma}(\omega_2) \rangle = \frac{2\pi(4\alpha - i\omega_1 - i\omega_2)\delta(\omega_1 + \omega_2)}{(2\alpha - i\omega_1)(2\alpha - i\omega_2)}$$

$$\begin{aligned} \tilde{\mathcal{G}}_{l,m}(\omega) &= \sum_{s=1}^{N} \frac{\phi_s(l)\phi_s(m)}{\lambda_s + i\omega} \\ &= \frac{\sin(lq)\sin[(N-m+1)q]}{\sin q \sin[(N+1)q]} \end{aligned}$$

where $\lambda_s = 2[1 - \cos(s\pi/(N+1))]$,

$\phi_s(l) = \sqrt{2/(N+1)}\sin(sl\pi/(N+1))$

Mean-squared displacement:

$$\Delta_l(t) = \mathcal{C}_{l,l}(t) = \frac{2v_0^2\alpha}{\pi}\int_{-\infty}^{\infty} \frac{\sum_k \tilde{\mathcal{G}}_{l,k}(\omega)\ \tilde{\mathcal{G}}^T_{l,k}(-\omega)}{4\alpha^2+\omega^2}(2-2\cos\omega t)\ d\omega\,.$$

$$\Delta(t) = \frac{1}{N}\sum_{l=1}^{N}\Delta_l(t)$$
$$= \frac{2v_0^2\alpha}{\pi}\int_{-\infty}^{\infty}\mathcal{B}(\omega)\frac{(2-2\cos\omega t)}{(4\alpha^2+\omega^2)}\ d\omega,$$

$$\mathcal{B}(\omega) = \frac{1}{N}\mathrm{Tr}\left[\tilde{\mathcal{G}}_{l,m}(\omega)\tilde{\mathcal{G}}_{m,l}(-\omega)\right]$$
$$= 2\ \mathrm{Re}\left[\frac{1}{2\omega\sqrt{\omega^2-4ik\omega}}\right]$$

Different time regimes:

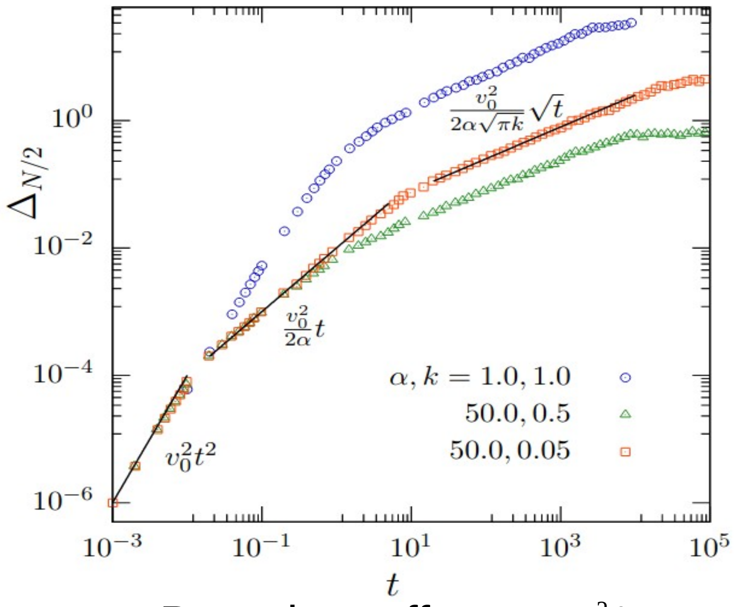
$t \ll \alpha^{-1}, k^{-1}$ $\quad \Delta_{N/2}(t) = v_0^2 t^2\left(1+\mathcal{O}(\alpha t)\right)$

$\alpha^{-1} \ll t \ll k^{-1}$ $\quad = 2D_{\text{eff}}t$

$t \gg \alpha^{-1}, k^{-1}$ $\quad = 2D_{\text{eff}}(\pi k)^{-1/2}t^{1/2},$

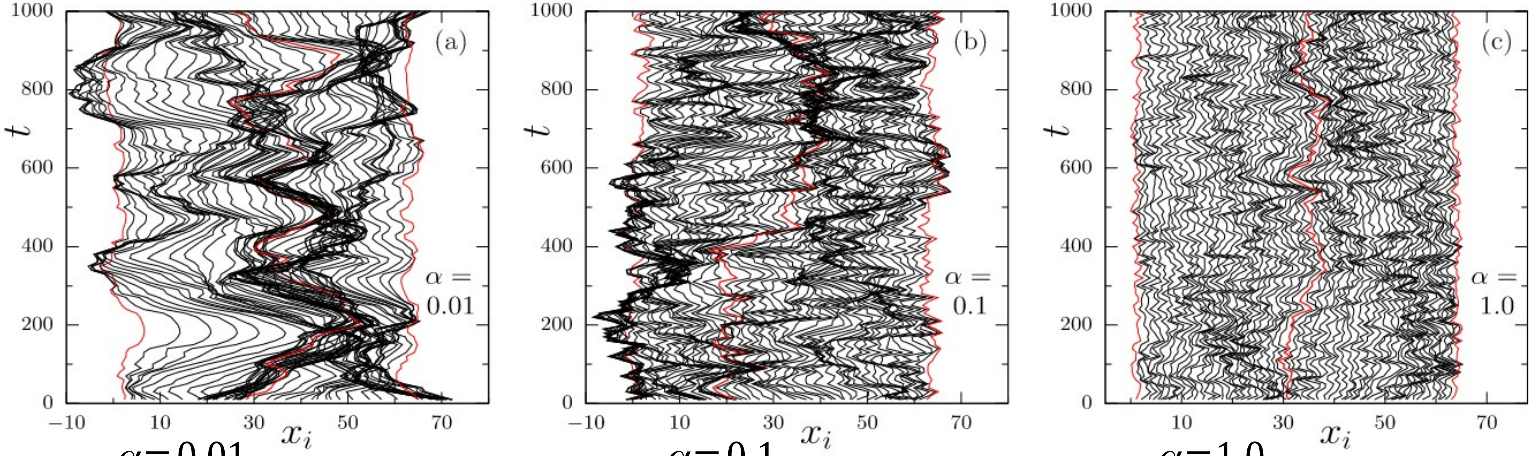
with $D_{\text{eff}} = v_0^2/2\alpha.$

Also, $(\rho v_0)^{-1} = \gamma/K$



Boundary effects $\sim N^2/k$

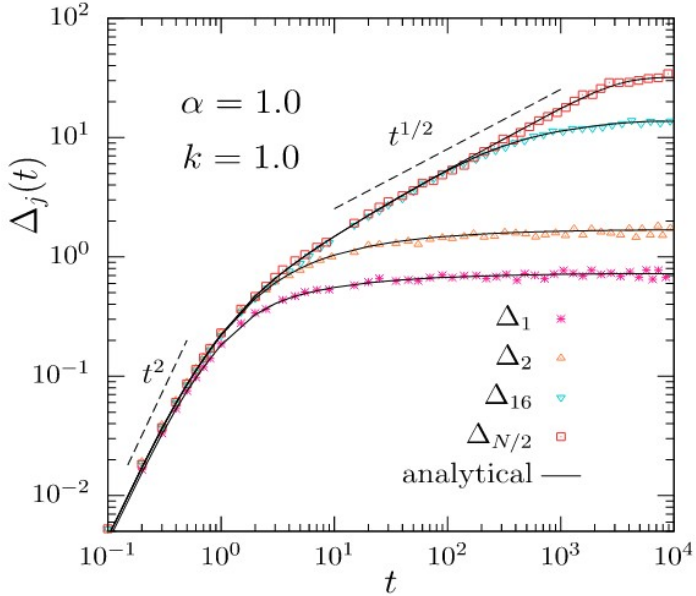
Trajectories:



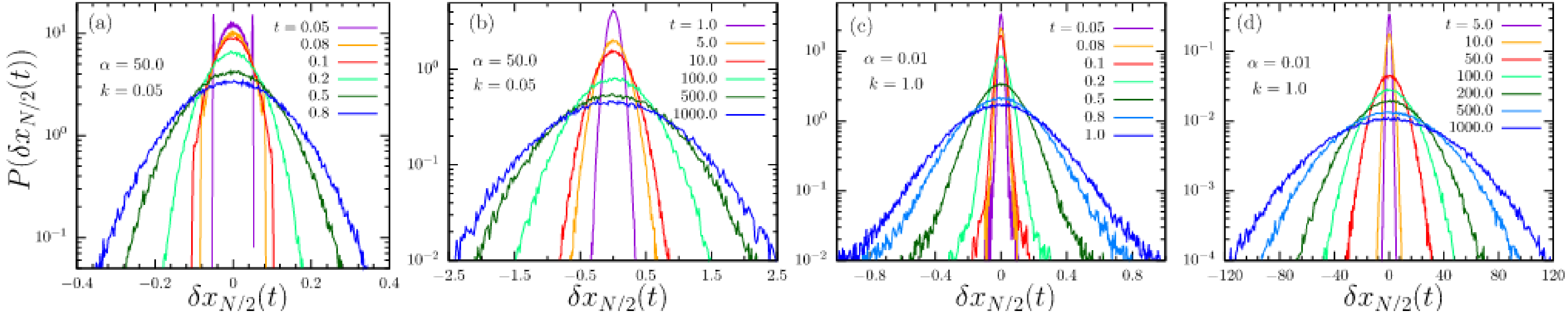
$\alpha = 0.01$ $\alpha = 0.1$ $\alpha = 1.0$

Due to boundary pinning, tagged particle dynamics will be different as one approaches from bulk to boundary.

$$\Delta_l(t) = \mathcal{C}_{l,l}(t) = \frac{2v_0^2\alpha}{\pi}\int_{-\infty}^{\infty} \frac{\sum_k \tilde{\mathcal{G}}_{l,k}(\omega)\ \tilde{\mathcal{G}}^T_{l,k}(-\omega)}{4\alpha^2+\omega^2}\,(2-2\cos\omega t)\ d\omega\,.$$



Evolution of distribution: $P(\delta x_{N/2}, t), \quad \delta x_{N/2}(t) = x_{N/2}(t) - x_{N/2}(0).$

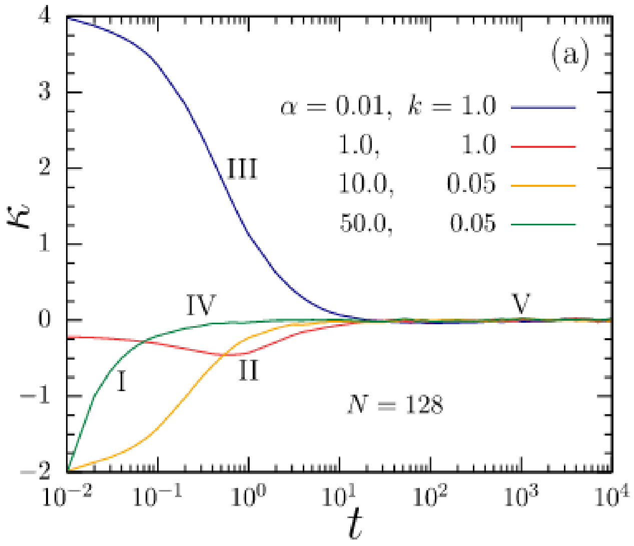


$\alpha^{-1} = 0.02\,, k^{-1} = 20.0$

$\alpha^{-1} = 100.0\,, k^{-1} = 0.01$

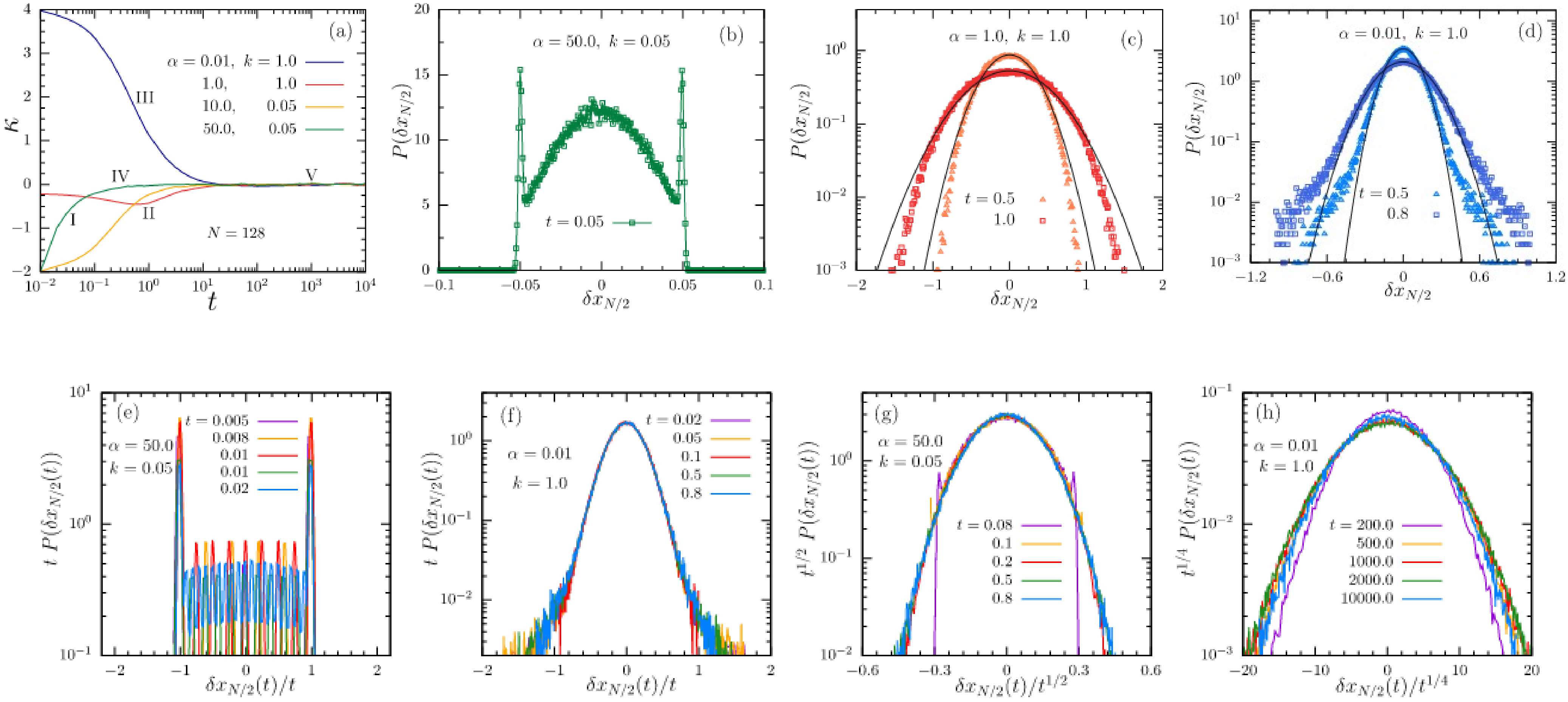
Excess kurtosis:

$$\kappa(t) = \frac{\left\langle \left[\delta x_{N/2}(t) - \mu(t)\right]^4 \right\rangle}{\left\langle \left[\delta x_{N/2}(t) - \mu(t)\right]^2 \right\rangle^2} - 3.0\,,$$



$II \rightarrow \alpha^{-1}$

Kurtosis and deviations from a Gaussian:



ballistic   ballistic   diffusive   sub-diffsive

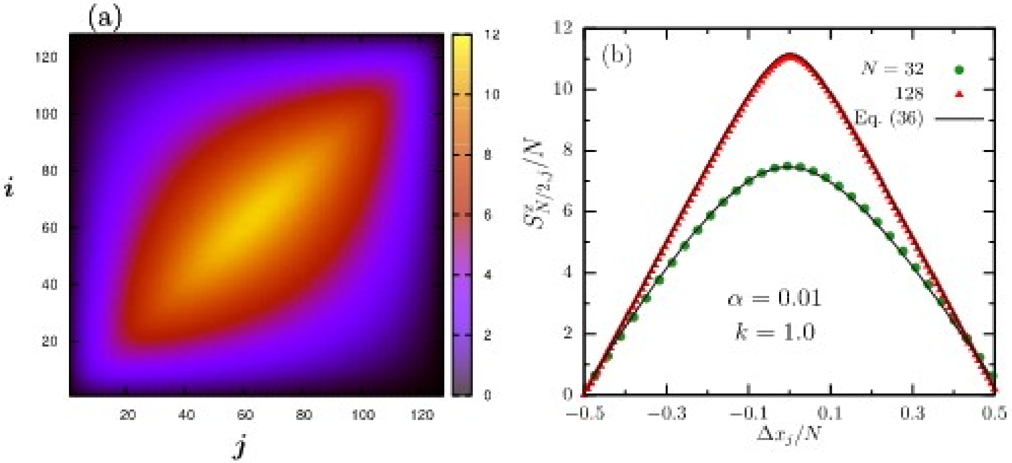
Equal-time correlations:

$$S^x_{l,m} = v_0^2 \sum_{s=1}^{N} \frac{\phi_s(l)\phi_s(m)}{\lambda_s(2\alpha+\lambda_s)} = \frac{2v_0^2\alpha}{\pi}\int_{-\infty}^{\infty} \frac{F_{l,m}(\omega)}{4\alpha^2+\omega^2}\, d\omega\,,$$

$$F_{l,m}(\omega) = -\frac{1}{\omega}\mathrm{Im}\left[\frac{\sin(lq)\sin(N-m+1)q}{\sin(q)\sin((N+1)q))}\right] \quad \text{for} \quad l \le m$$

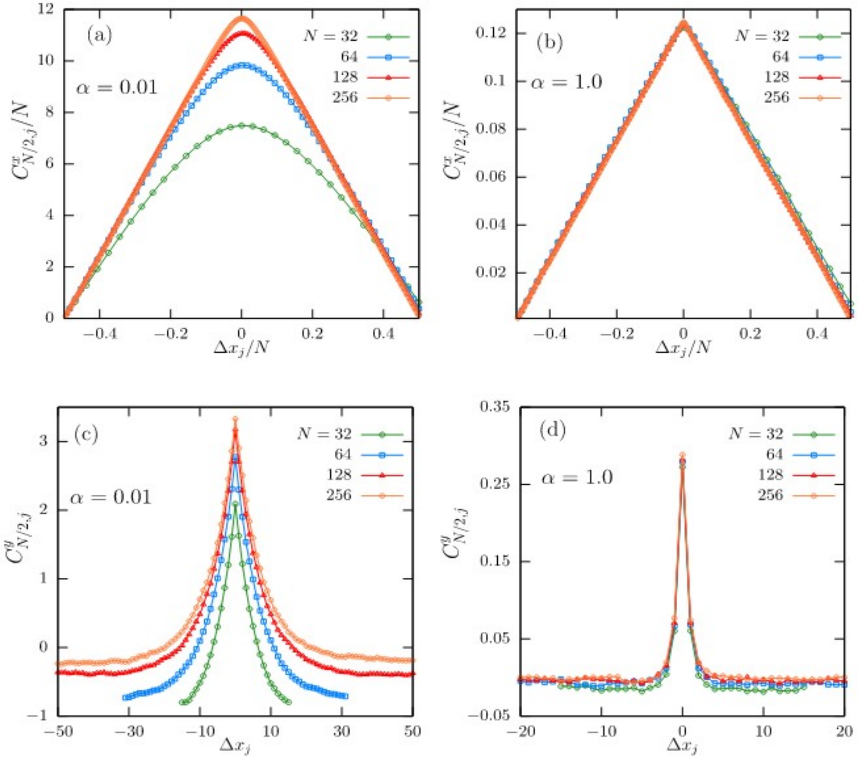
$$F_{l,m}(\omega) = \left[\sum_k \tilde{\mathcal{G}}_{l,k}(\omega)\ \tilde{\mathcal{G}}^T_{m,k}(-\omega)\right]$$

becomes sharply peaked at $\omega = 0$ as N increases.



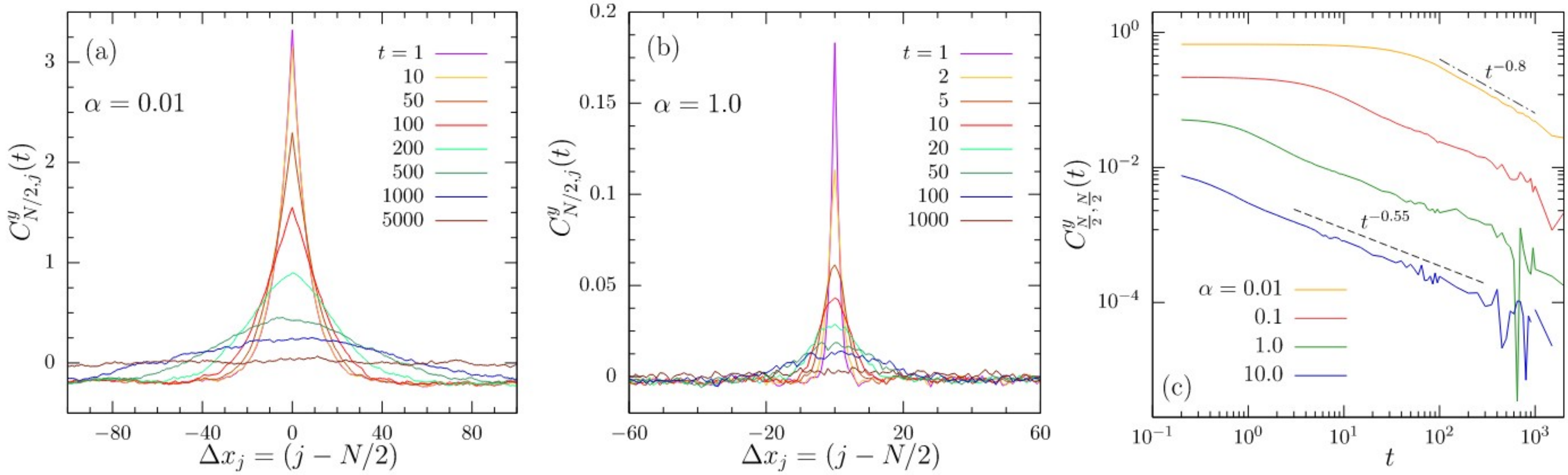
Now, in the large α limit:

$$S^{x(\mathrm{eq})}_{l,m} = k_B T(\Phi^{-1})_{l,m} = \frac{k_B T}{k}\frac{l(N-m+1)}{(N+1)}\,, \quad \text{for} \quad m > l$$



$$S^y_{i,j} = \lim_{t_0\to\infty}\langle y_i(t_0)y_j(t_0)\rangle\,, \qquad y_l(t) = x_{l+1}(t) - x_l(t)$$

Two-time correlations:



- Diffusive spreading of auto-correlation for higher α
- The exponent changes as the activity increases.

Summary

- We have obtained a closed-form expression for MSD and correlations for a linear chain of RTPs.

- From the MSD, depepnding upon the choice of time scales as well as their separations (persistence time α^{-1} and the interaction time k^{-1}), one can get various behavior. However, the late time $t \gg \alpha^{-1}, k^{-1}$ sub-diffusive behavior is quite generic.

- The scaling of the two-point static correlation for displacement as well as for stretch shows signature of activity. For large α or in large N limit they converge to the equilibrium-like behavior.

- The decay ofthe autocorrelation for the stretch variable for the active case is faster than the diffusive behavior.

- The evolution of the probability distributions show non-Gaussian at early ($t < \alpha^{-1}, k^{-1}$) times which is also reflected by +ve or -ve values of kurtosis.

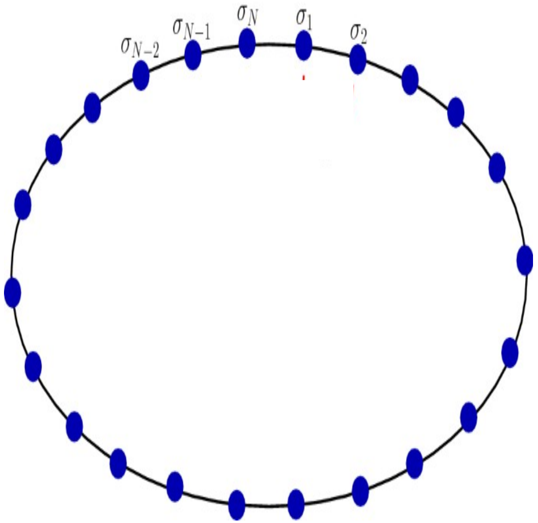
- Can be observed for other active particle models as well.

Thank you..

A few earlier Works:

P Singh, A Kundu, J. Phys. A: Math Theor. 54 305001 (2021)
S Put et al, J. Stat. Mech. 123205 (2019)

- Considered Rouse model with telegraphic noise
- Variance and two-point correlations in terms of the sum of modes
- Considered $\tau_K \ll \tau_A \ll \tau_N$
- Showed a ballistic to super-diffusive to SFD crosovers.
- Obtained scaling forms for two-point as well as auto-correlations.



P Dolai et al., Soft Matter, 16, 7077 (2020).

- WCA type of interaction among the active particles.
- Interaction time-scale depends upon density of particles
- Tagged particle dynamics shows crossover from ballistic to a single-file-diffusion.

Recent interests in collective behavior in active lattice gas models as well (microscopic as well as hydrodynamics).