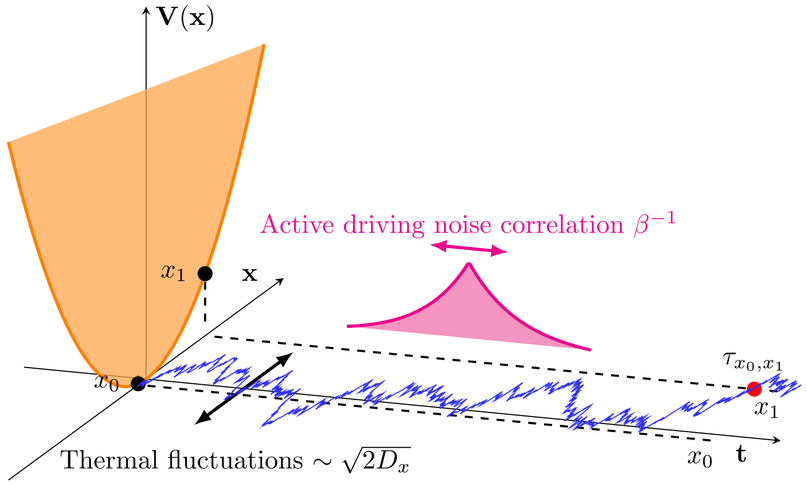
First-passage times of thermal active particles*

@MPI-PKS Dresden // 16th Sep 2020



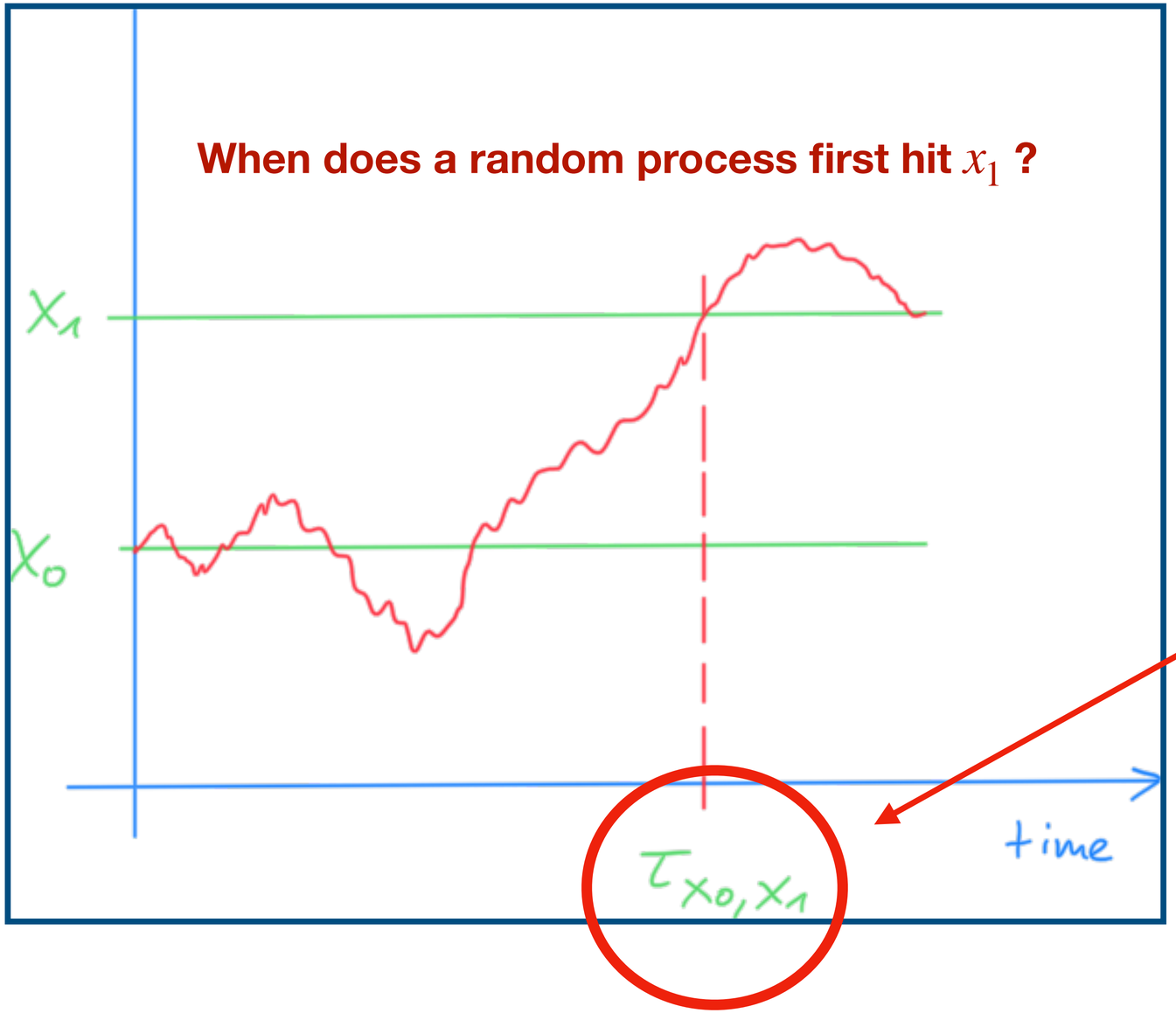
Benjamin Walter (Imperial College London) [b.walter16@imperial.ac.uk]

***Joint work with Gunnar Pruessner and Guillaume Salbreux, arXiv:2006.00116**

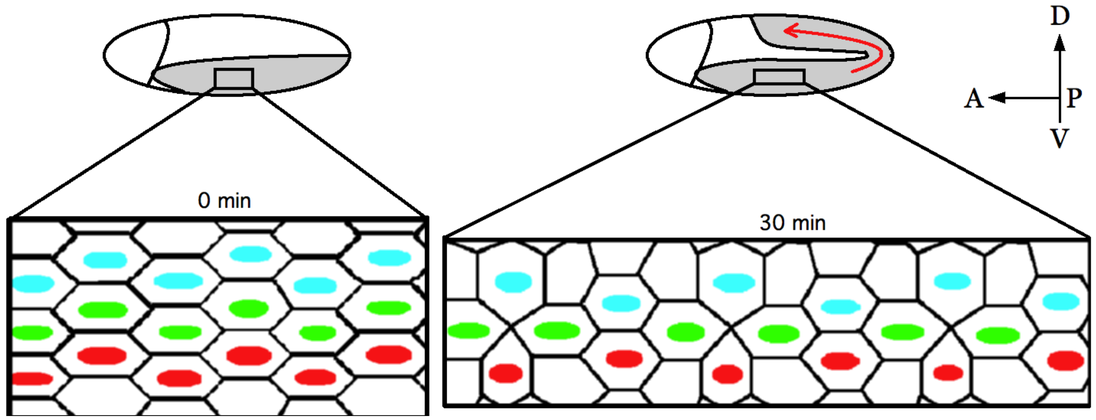
Outline

- First-passage times in biophysics and beyond
- The problem of memory
- Thermal active particles
- Perturbative Solution to First-passage time problem

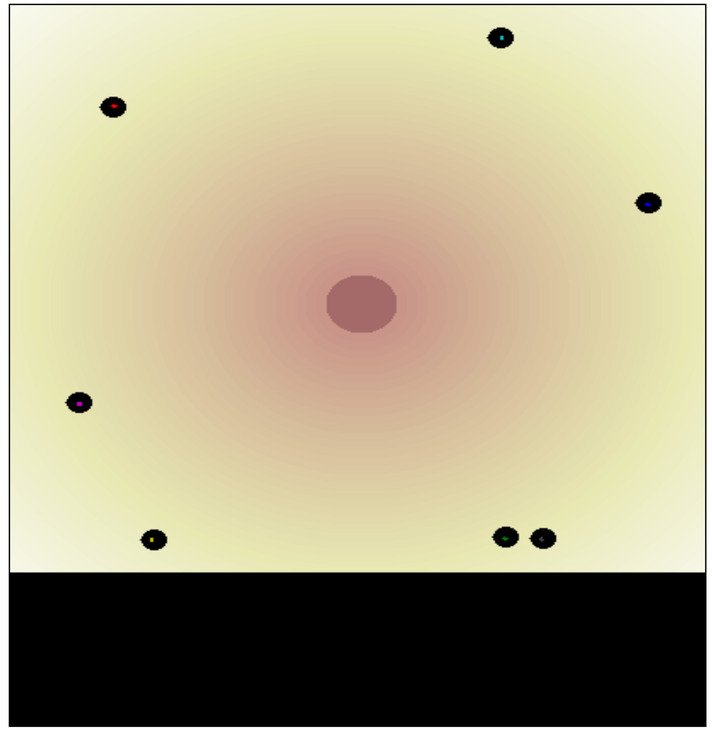
First-passage times



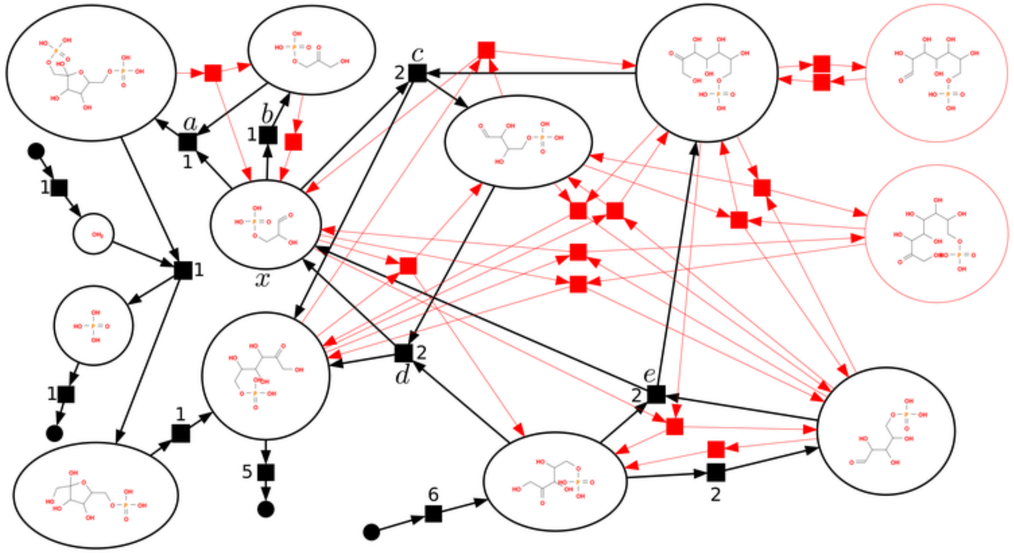
First-passage times everywhere



Germ-band extension



Bacterial search



Chemical Reaction Networks

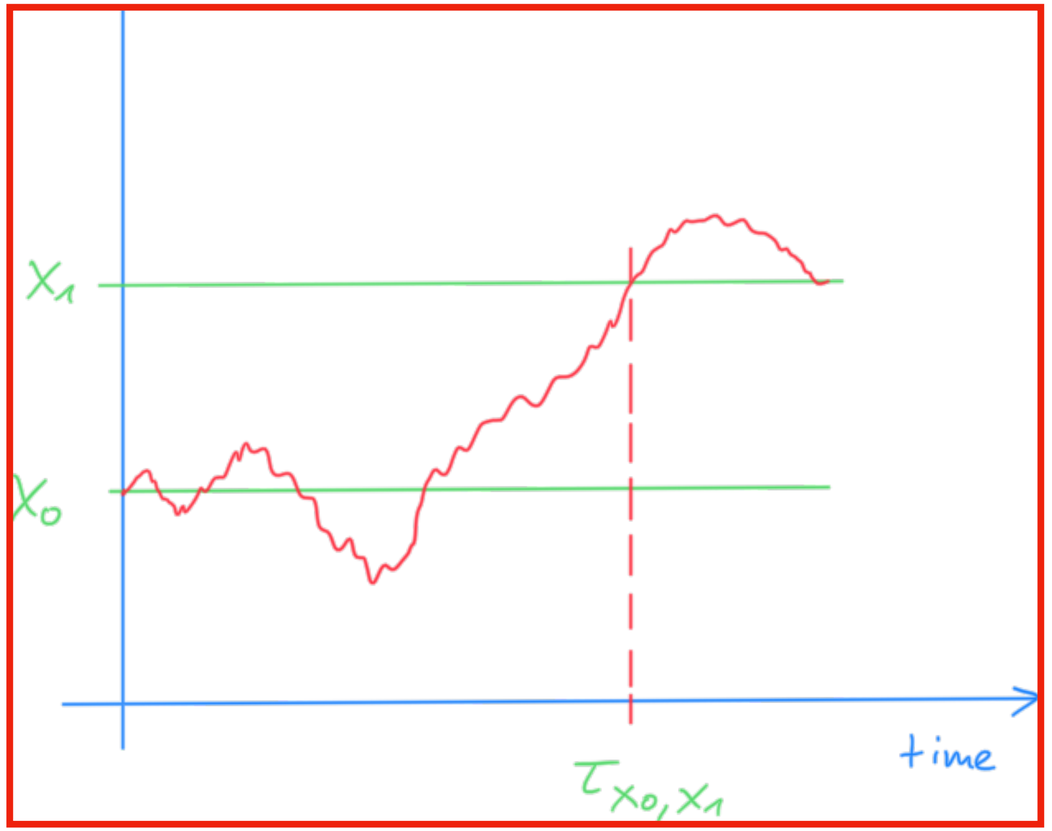
First-passage time distributions reveal

- Chemical reaction dynamics (protein assembly, neuron activity,…)
- Mechanical properties of active tissues (embryonic development, cancer growth,…)
- Diffusion in non-heterogeneous media (on networks, single-file diffusion,…)
- Safety in mechanical engineering (cracking, fault propagation)
- Finance (option pricing)

Key characteristic for complex systems

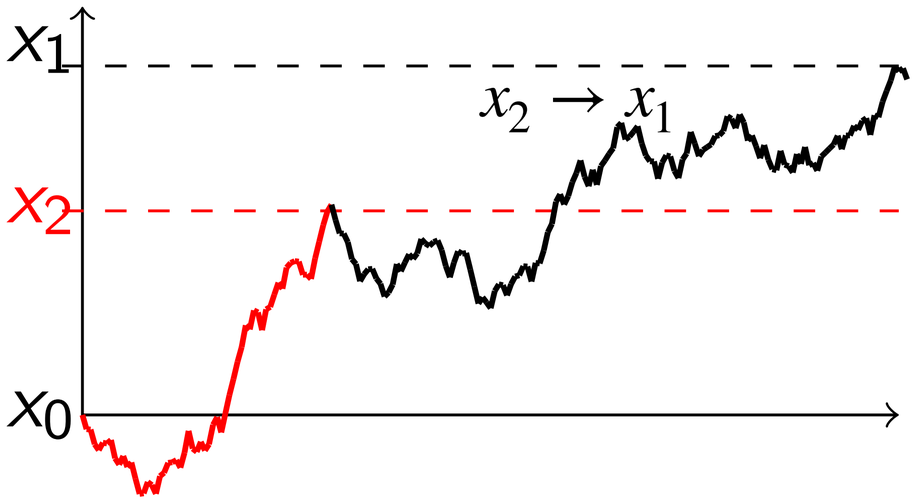
The first-passage time *problem*

- Global observable τ_{x_0,x_1} (keep track of entire path $x(t)$)
- Full distribution $F(\tau_{x_0,x_1})$ only for simplest cases
- 100+ years of research
- Most often: *Mean* first passage time



Markovian first-passage times

- No memory, no problem (*D. A. Darling, A. J. F. Siegert*, PR 1953)



Transition probability

$$T(x_0 \to x_1, t) = (F(x_0 \to x_2) * T(x_2 \to x_1))[t]$$

First-passage time prob.

Laplace Transform

$$F(s) = \frac{T(x_0 \to x_1; s)}{T(x_1 \to x_1, s)}$$

Return probability

$F(s) = \int_0^\infty \mathrm{d}\tau\, e^{-\tau s} F(\tau)$ **is the moment generating function**

$$F(s) = 1 - \langle \tau \rangle + \frac{1}{2} \langle \tau^2 \rangle - \dots$$

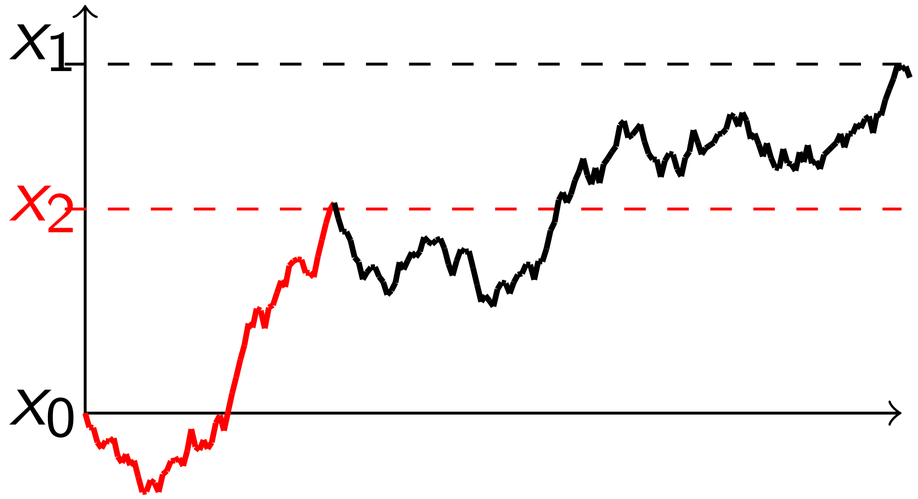
Markovian first-passage times

- Find transition probabilities, obtain all moments of first-passage time distribution

$$\partial_t T(x_0, x_1) = \mathscr{L} T(x_0, x_1)$$

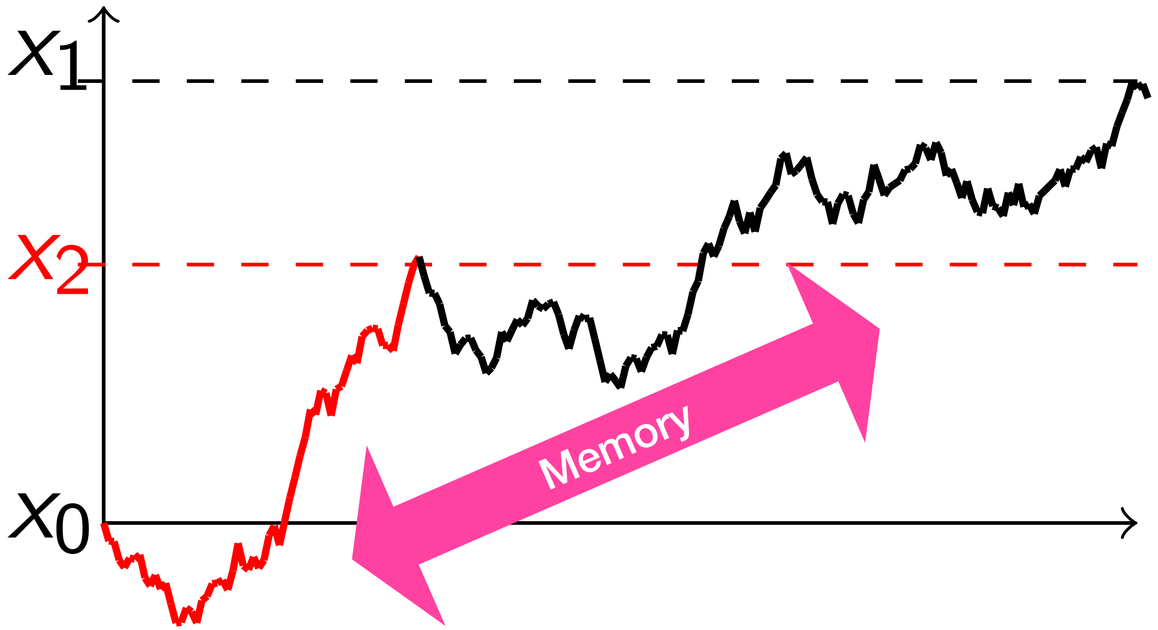
Fokker Planck Equation

$$F(s) = \frac{T(x_0 \to x_1; s)}{T(x_1 \to x_1, s)}$$



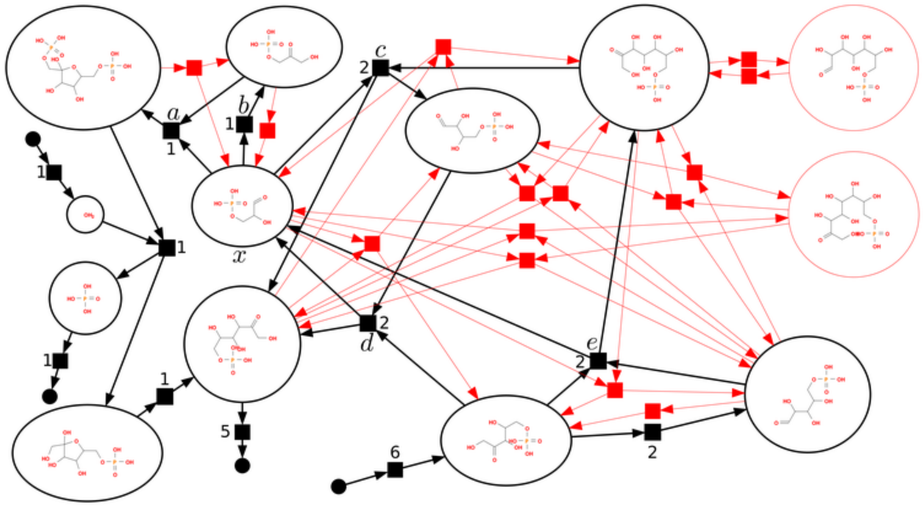
For Markov processes, finding first-passage times = Solving a partial differential equation

Non-markovian processes?

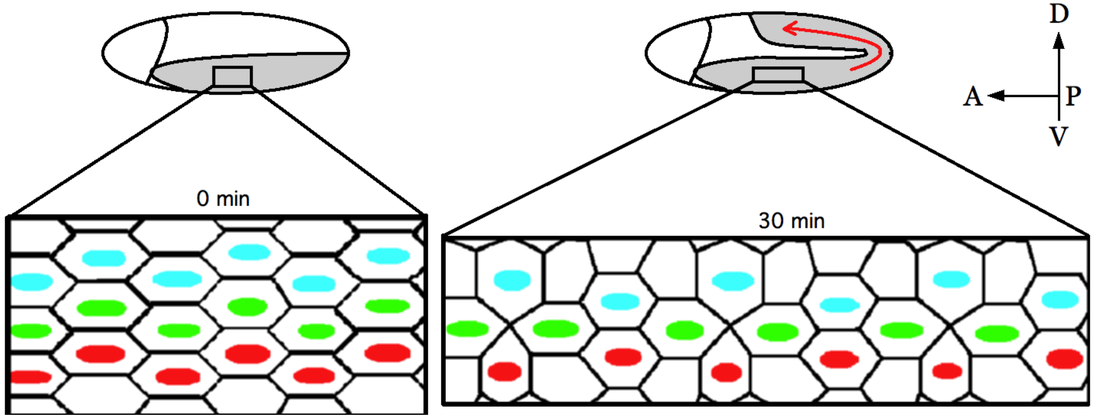


Renewal approach no longer valid

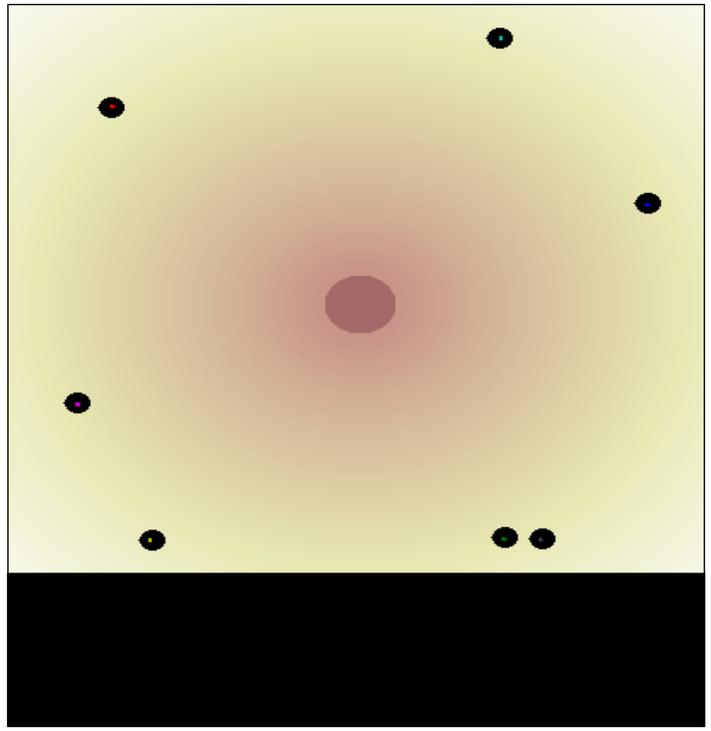
Nothing is Markovian



Chemical Reaction Networks



Germ-band extension



Aim

- Find first passage time distribution for relevant Non-Markovian processes *perturbatively*

Short-range memory

Thermal Active Processes

Long-range memory

Fractional Brownian Motion

M Arutkin, B Walter, K J Wiese. PRE 102, 022102 (2020)

B Walter, K J Wiese. PRE 101, 043312 (2020)

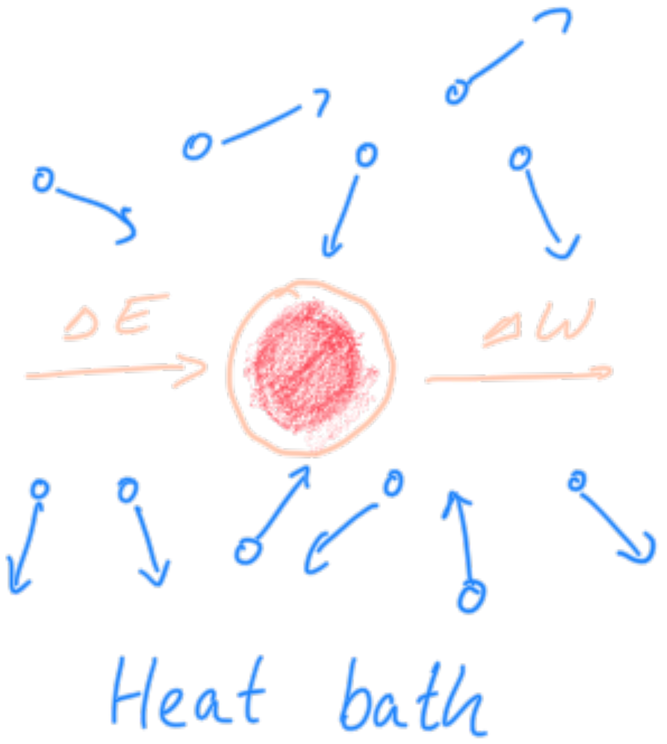
Thermal Active Matter in Potential

- Particle coupled to heat bath
- Actively self-propelling
- Subject to potential force

$$\dot{x}_t = -V'(x_t) + \xi_t + \varepsilon y_t$$

$$\langle \xi_t \xi_s \rangle = 2D_x \delta(t-s)$$

$$\langle y_t y_s \rangle = D_y \beta^{-1} \exp\left(-\beta\,|\,t-s\,|\right)$$



L. Caprini, U. M. B. Marconi, A. Puglisi, and A. Vulpiani, JSM 053203 (2019)
F. J. Sevilla, R. F. Rodríguez, and J. R. Gomez-Solano. PRE 100, 032123 (2019)
L. Dabelow, S. Bo, and R. Eichhorn, PRX 9, 021009 (2019)

Thermal Active Matter in Potential

Perturbation Theory

$$\dot{x}_t = -V'(x_t) + \xi_t + \varepsilon y_t$$

Key Idea
Given one knows moment generating function for $\varepsilon = 0$,
one can find systematic corrections for $\varepsilon \neq 0$.

$$\mathscr{M}(s) = \left\langle e^{-s\tau_{x_0,x_1}} \right\rangle = \mathscr{M}_0(s) + \varepsilon^2 \mathscr{M}_1(s) + \dots$$

Darling-Siegert

non-Markovian correction

Thermal Active Matter in Potential

Technical arguments

$$\mathscr{M}(s) = \left\langle e^{-s\tau_{x_0,x_1}} \right\rangle = \mathscr{M}_0(s) + \varepsilon^2 \mathscr{M}_1(s) + \dots$$

$$\mathscr{M}_1(s) = \left\langle \iint \mathrm{d}s_1 \mathrm{d}s_2 \left. \frac{\delta \mathscr{M}(s)}{\delta y_{s_1} \delta y_{s_2}} \right|_{y \equiv 0} y_{s_1} y_{s_2} \right\rangle_y$$

Response functional of moment generating function

$$\left. \frac{\delta \mathscr{M}(s)}{\delta y_{s_1} \delta y_{s_2}} \right|_{y \equiv 0} = \left. \frac{\delta}{\delta y_{s_1} \delta y_{s_2}} \frac{T(x_0 \to x_1)}{T(x_1 \to x_1)} \right|_{y \equiv 0}$$

Response functional of transition probabilities

arXiv:2006.00116

Thermal Active Matter in Potential

Technical arguments

How to find $\left.\frac{\partial}{\partial y_{s_1}} T(x_0 \to x_1)\right|_{y\equiv 0}$, $\left.\frac{\partial}{\partial y_{s_1}\partial y_{s_2}} T(x_0 \to x_1)\right|_{y\equiv 0}$, … ?

Diagonalise Fokker Planck equation

$$\partial_x(V'(x)u_n(x)) + D_x\partial_x^2 u_n(x) = -\lambda_n u_n(x) \qquad v_n(x) = \exp\left(V(x)/D_x\right) u_n(x) \qquad \lambda_n \geq 0$$

All functional derivatives can be expressed in terms of $u_n(x)$, $v_n(x)$, e.g.,

$$T(x_0 \to x_1) = \sum_n \frac{u_n(x_1)v_n(x_0)}{s+\lambda_n}, \dots$$

Integrate expressions over correlation kernel of y_t

For almost Markov processes, finding first-passage times = Diagonalising a partial differential operator

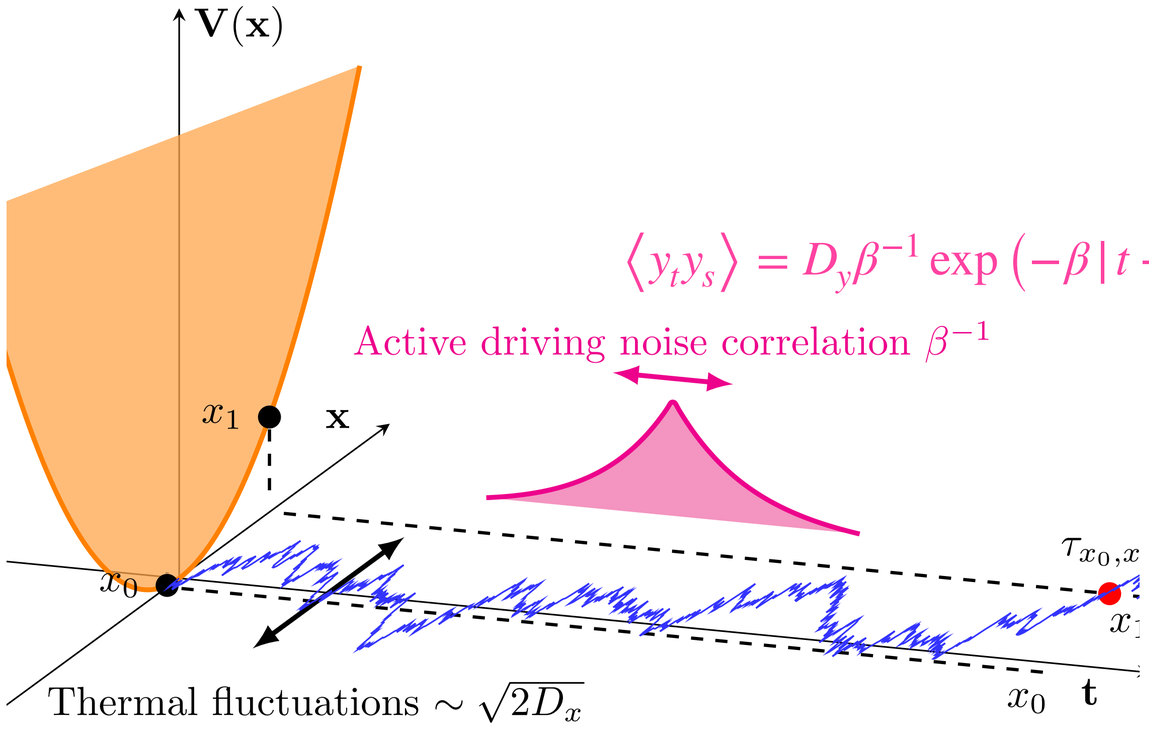
arXiv:2006.00116

For Markov processes, finding first-passage times = Solving a partial differential equation

Active Thermal Ornstein Uhlenbeck Process

1st Example

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



$$\langle y_t y_s \rangle = D_y \beta^{-1} \exp\left(-\beta\,|\,t-s\,|\right)$$

Active driving noise correlation β^{-1}

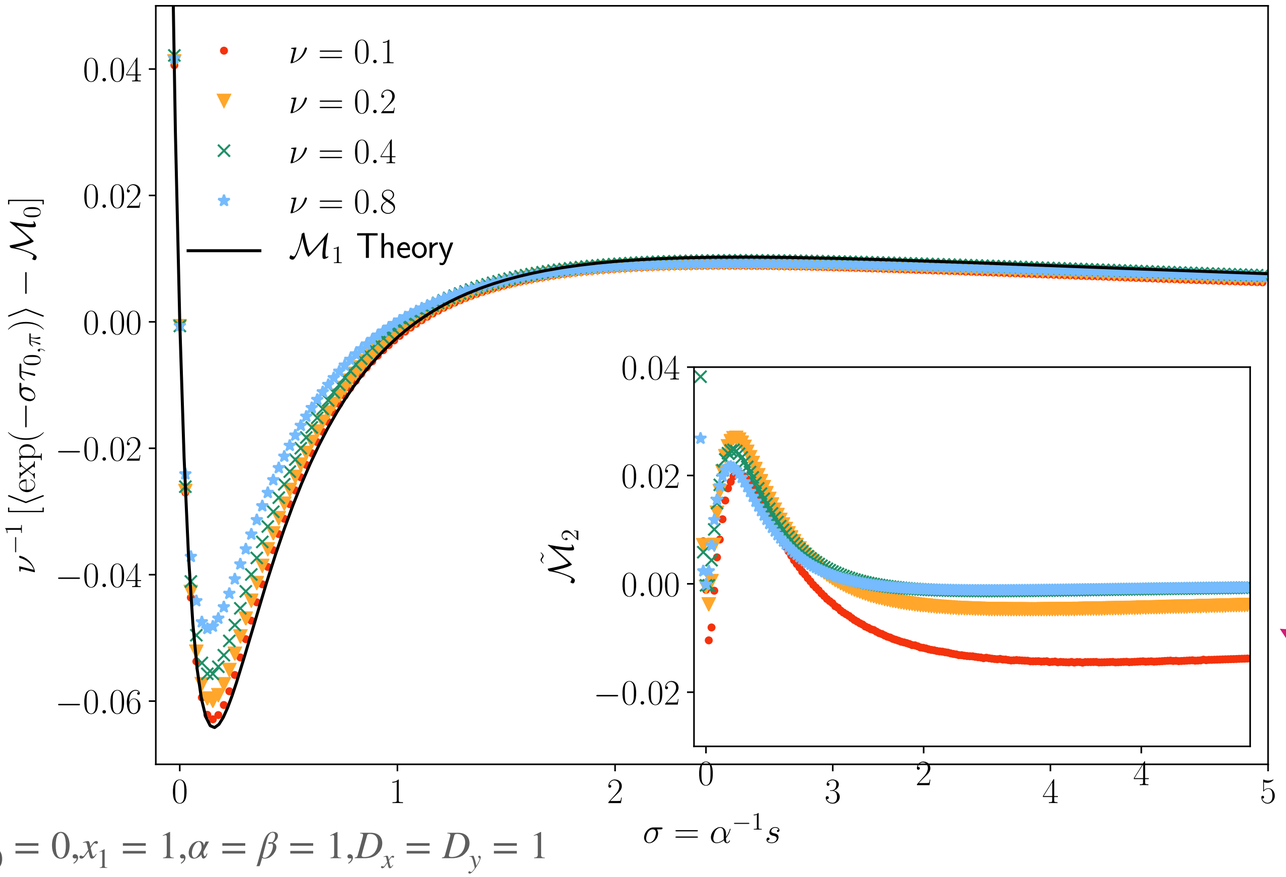
$$\dot{x}_t = -\alpha x_t + \xi_t + \varepsilon y_t$$

ATOU

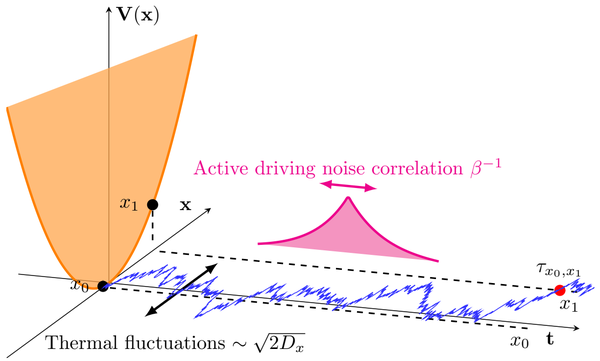
$$\nu = \frac{D_y \varepsilon^2}{D_x \alpha \beta}$$ **dimensionless perturbation parameter**

ATOU — Moment generating function

Measure $\dfrac{\tilde{\mathscr{M}}(s) - \mathscr{M}_0(s)}{\nu}$ and compare to analytically obtained first-order correction $\mathscr{M}_1(s)$



$x_0 = 0, x_1 = 1, \alpha = \beta = 1, D_x = D_y = 1$



ATOU

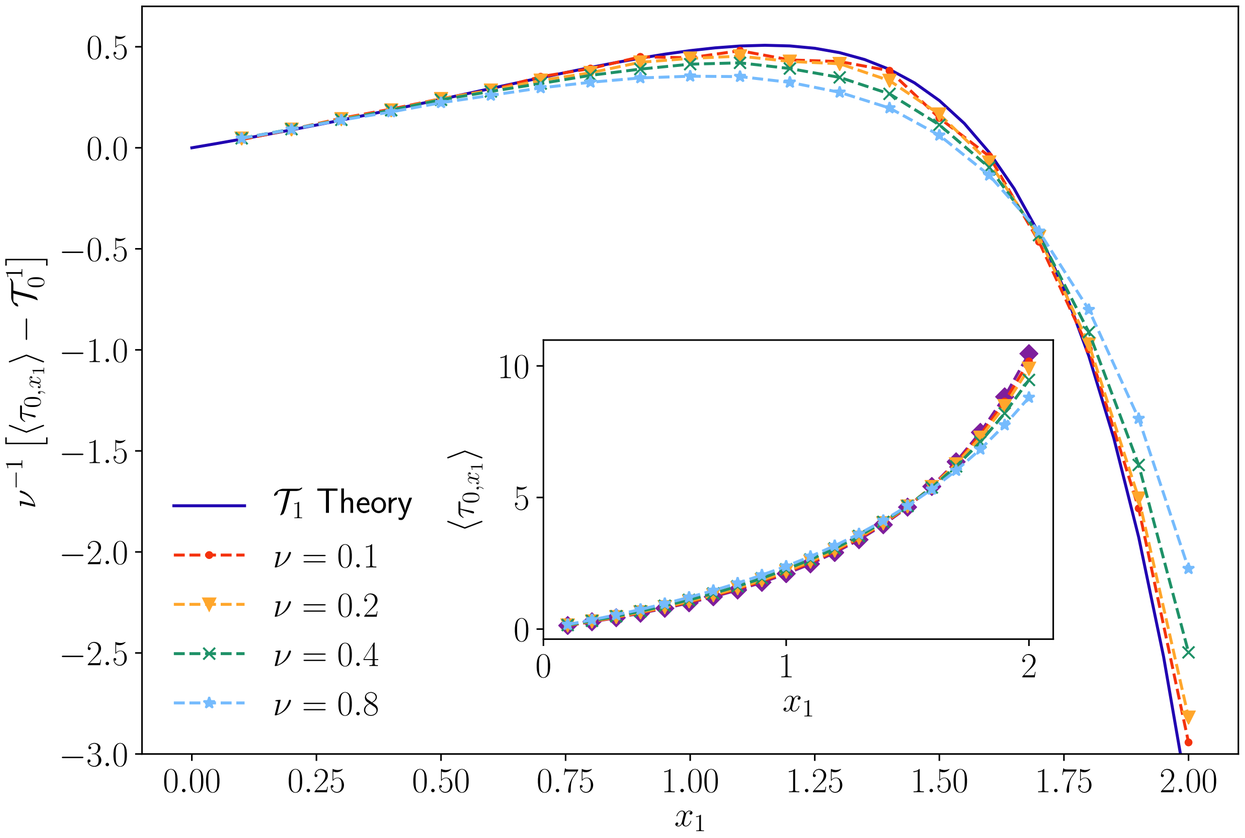
$$\mathscr{M}(s) = \left\langle e^{-s\tau_{x_0,x_1}} \right\rangle = \mathscr{M}_0(s) + \varepsilon^2 \mathscr{M}_1(s) + \dots$$

Systematic higher-order corrections

ATOU — Mean first passage time

Measure $\dfrac{\langle \tau(x_0 \to x_1) \rangle - \langle \tau(x_0 \to x_1) \rangle_0}{\nu}$ and compare to first-order correction $\mathcal{T}_1(s)$

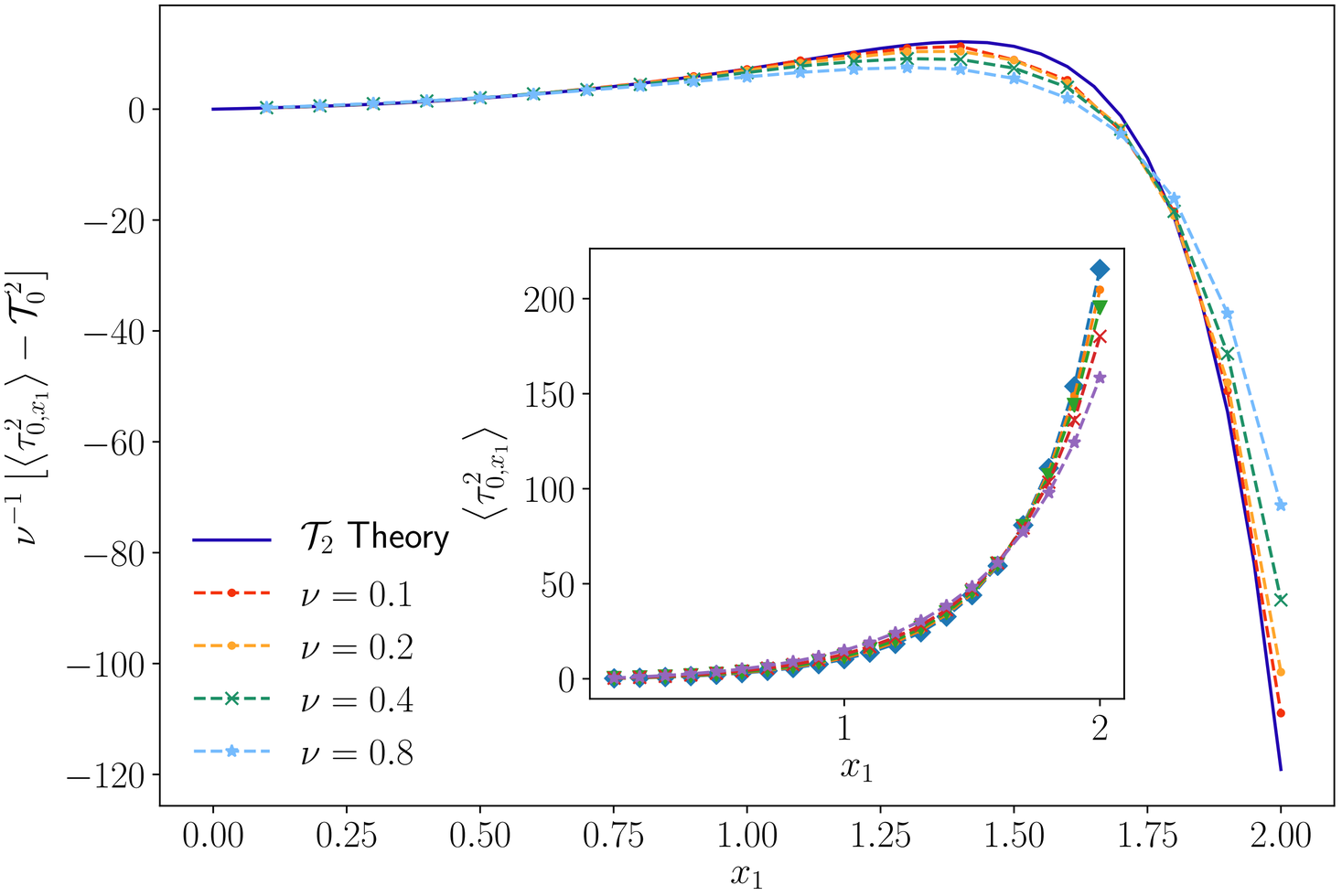
$$\langle \tau \rangle = -\frac{\partial}{\partial s} \mathcal{M}(s)$$



Additional driving noise slows down on short distances, speeds up on long distances

$x_0 = 0, \alpha = \beta = 1, D_x = D_y = 1$

ATOU — Second Moment of FPT



Measure

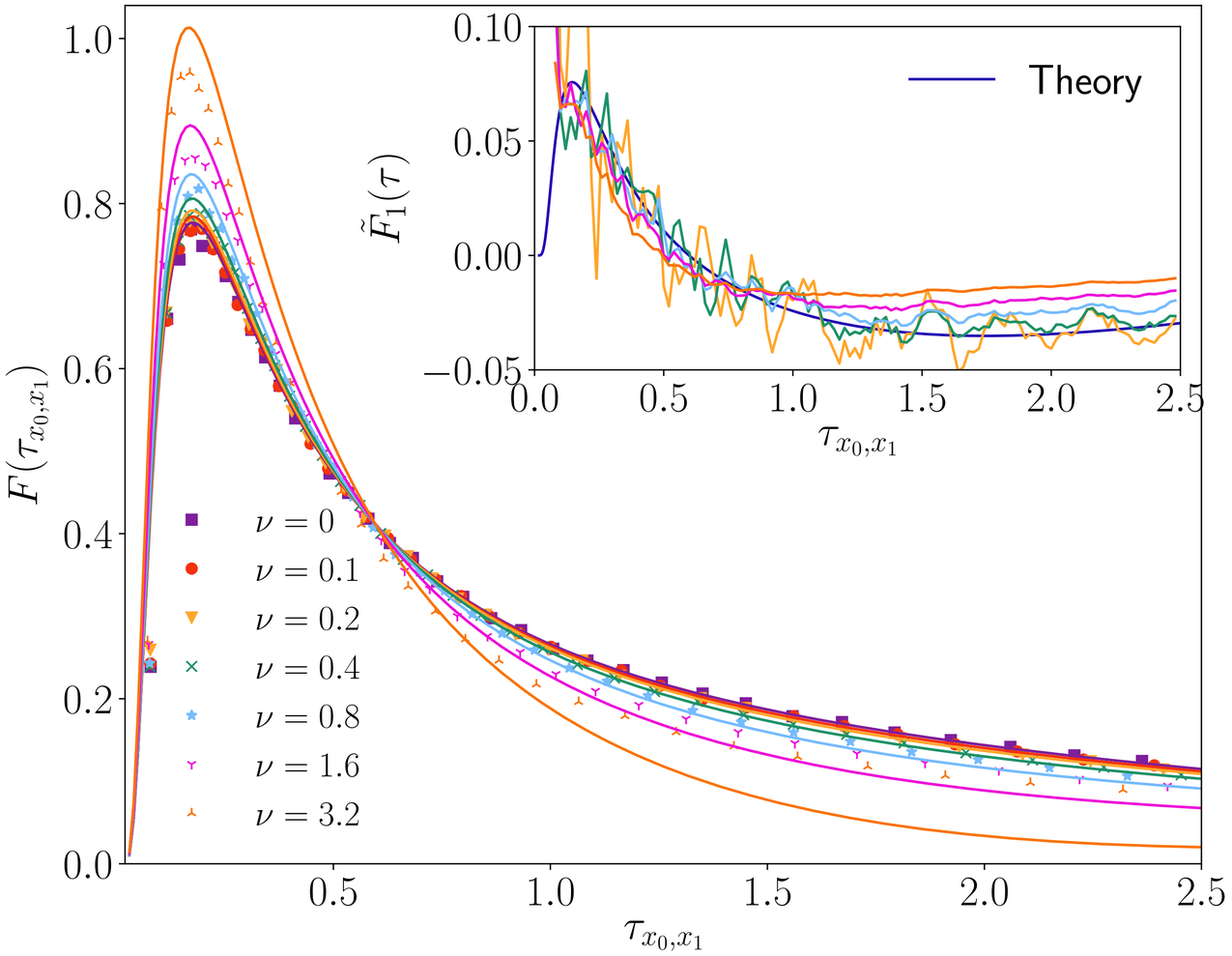
$$\frac{\left\langle \tau^2(x_0 \to x_1)\right\rangle - \left\langle \tau^2(x_0 \to x_1)\right\rangle_0}{\nu}$$

and compare to first-order correction

$$\mathcal{T}_2(s)$$

$$\left\langle \tau^2 \right\rangle = \frac{\partial^2}{\partial s^2}\mathcal{M}(s)$$

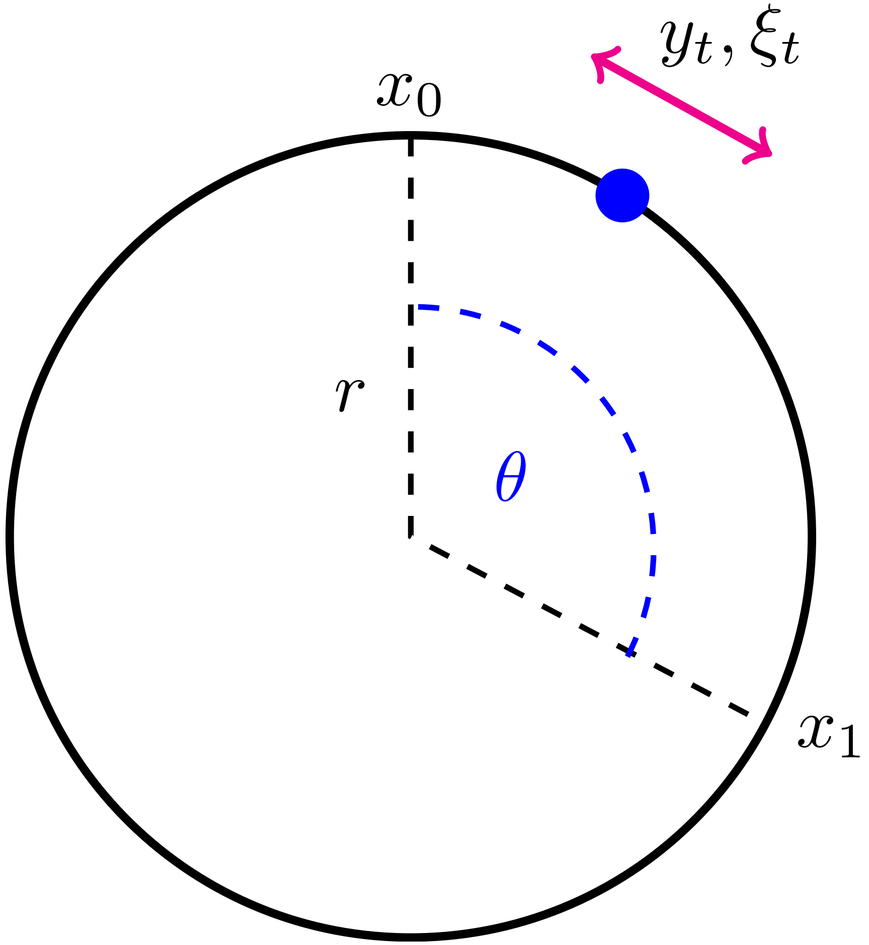
ATOU — Full distribution



Numerical Laplace inversion
From moment generating function to full distribution

Active Thermal Brownian Motion on a ring

2nd Example

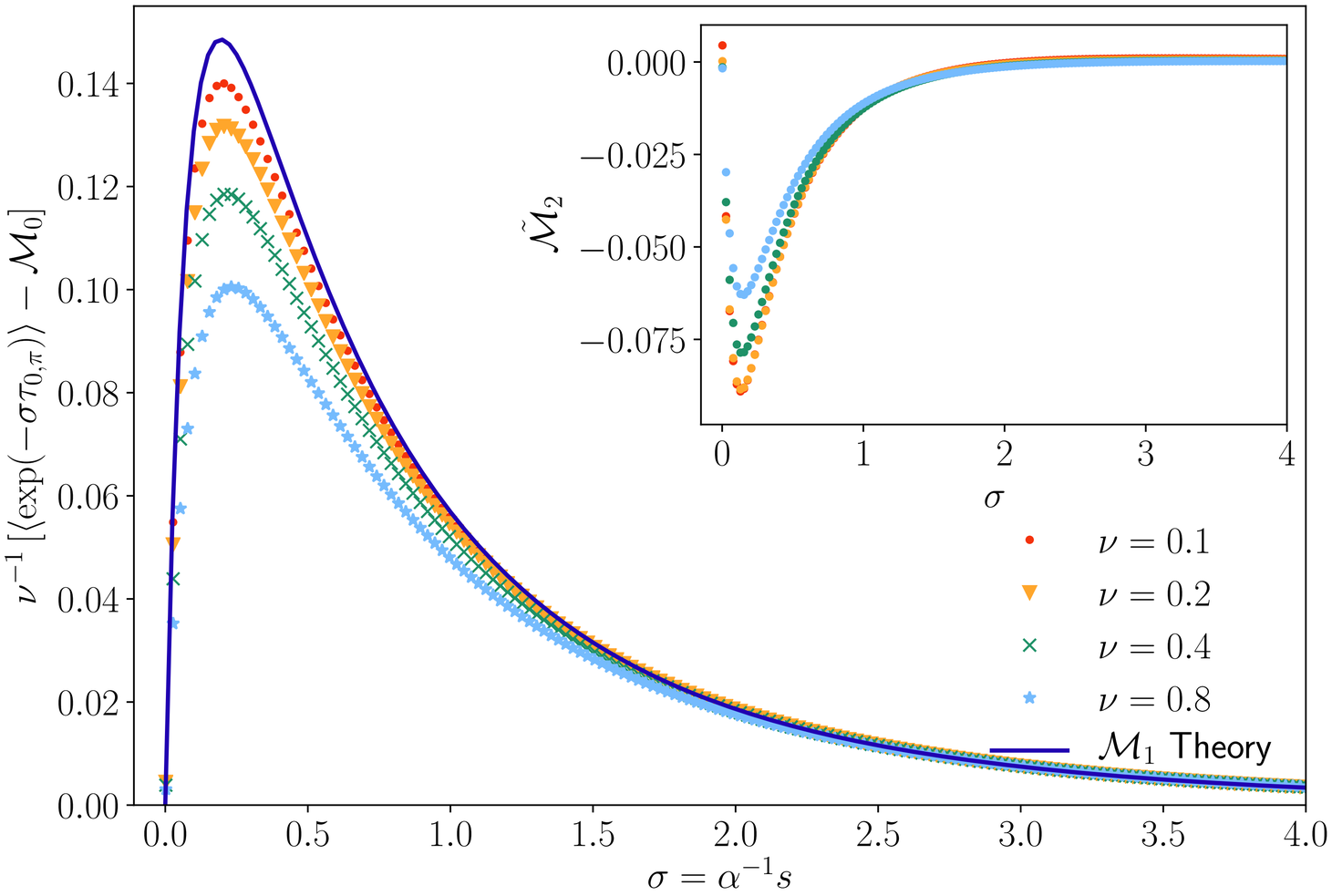


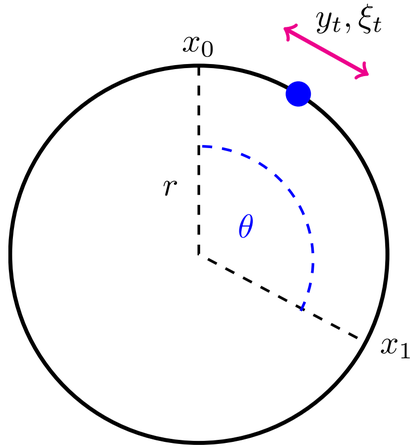
$$\langle y_t y_s \rangle = D_y \beta^{-1} \exp\left(-\beta\,|\,t-s\,|\right)$$

$$\dot{x}_t = \xi_t + \varepsilon y_t$$

$$\nu = \frac{D_y \beta r^2}{D_x^2}\varepsilon^2$$ **dimensionless perturbation parameter**

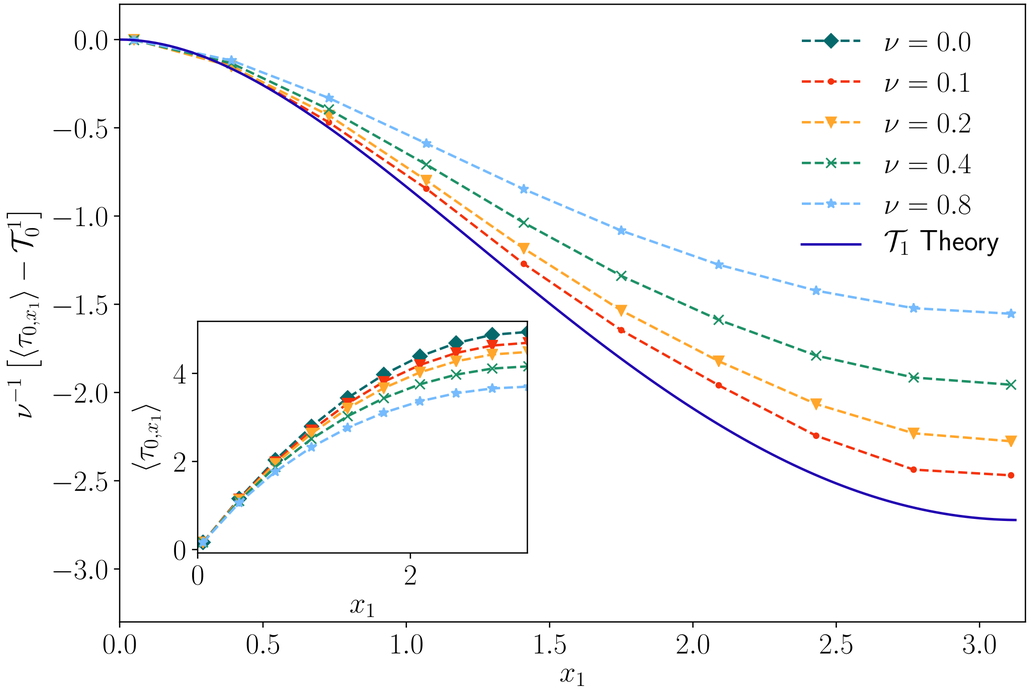
ATBM — Moment generating function



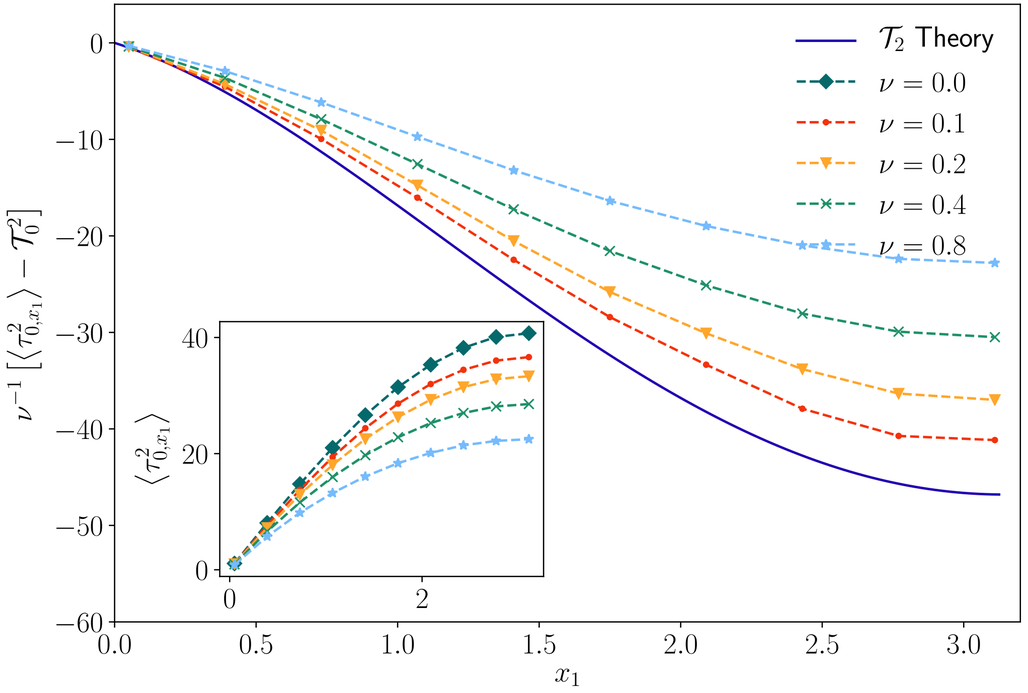


$x_0 = 0, x_1 = \pi, r = 1, \beta = 1, D_x = D_y = 1$

ATBM — First and Second Moment



First Moment

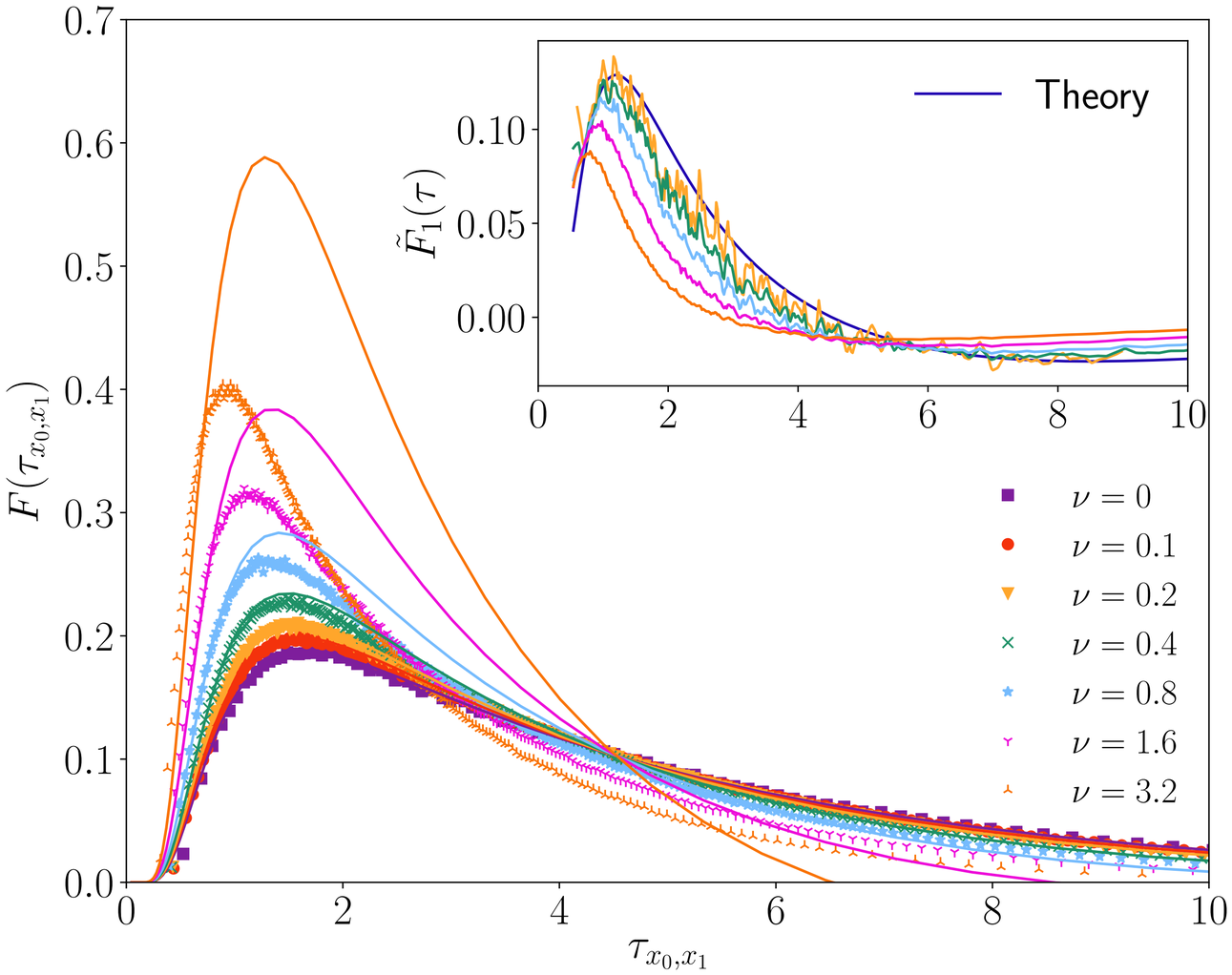


Second Moment

$$x_0 = 0, r = 1, \beta = 1, D_x = D_y = 1$$

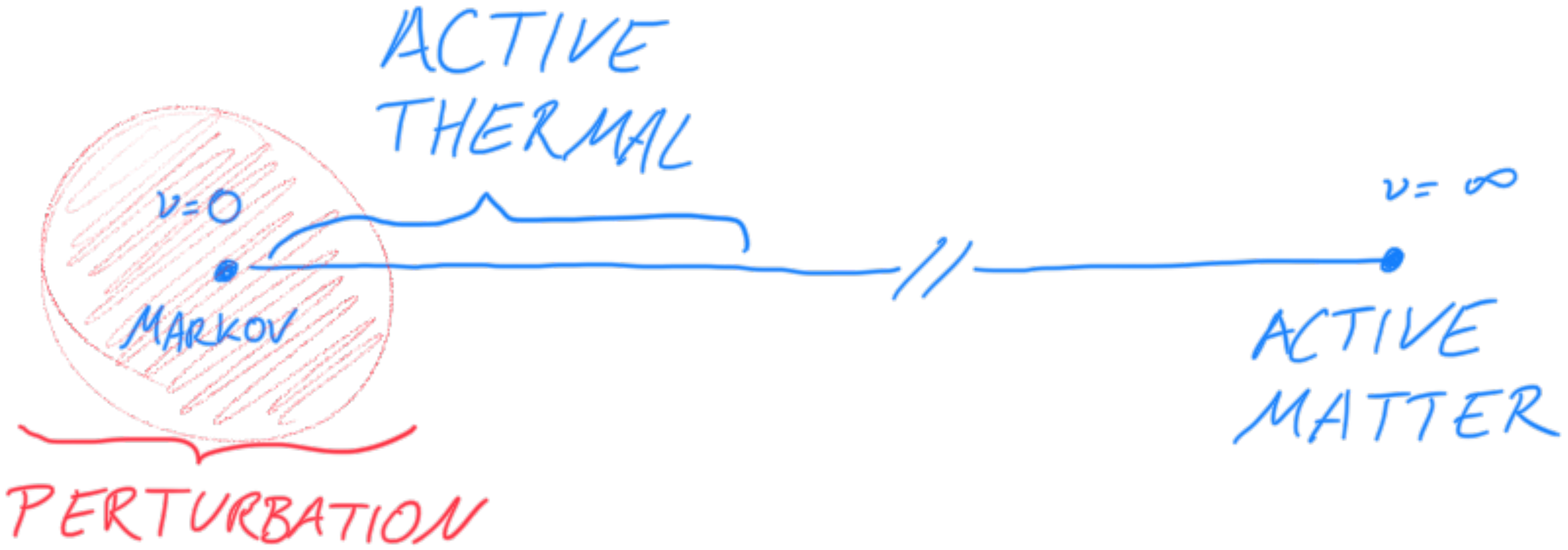
ATBM — Full distribution

Numerically inverted



Summary

- Active Thermal Processes interpolate between Markovian (thermal) and active processes
- The perturbative framework extends first-passage time tools from Markovian processes towards active matter

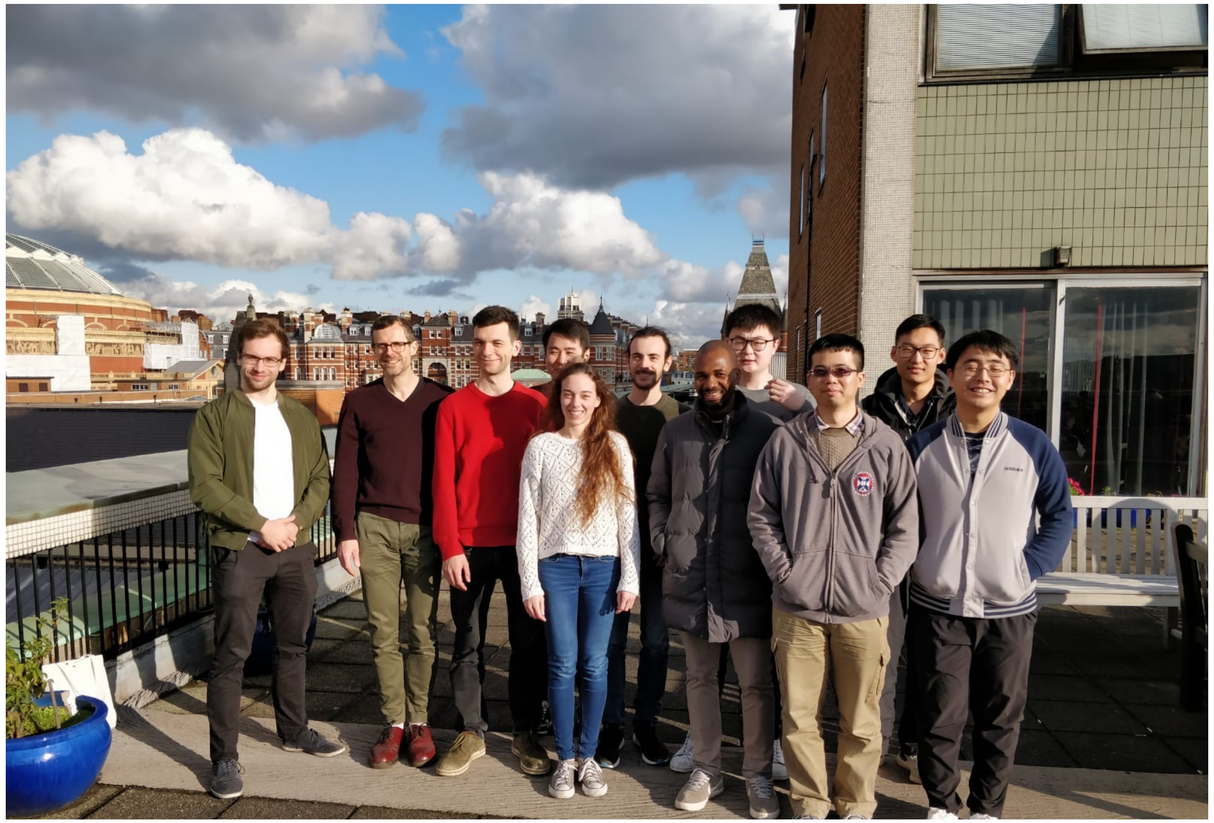


Summary

- **Systematic** and **controllable** expansion for **full** first-passage time statistics of non-Markovian stochastic process to arbitrary order in ν
- **No a-priori assumption on timescale of memory** (β), unlike other approximations (UCNA etc). (Quenched) limits $\beta \to 0, \infty$ allow study of disordered systems.
- Interplay of **heat bath, potential** and **memory** cast into mathematical framework with applications to other extreme values (running max, volume explored)

Acknowledgments!

- Gunnar Pruessner (ICL), Guillaume Salbreux (Francis Crick Institute)
- Nonequilibrium Group @ICL
- Kay Wiese, Gregory Schehr



Thank you for your attention, hospitality, and questions