Single file diffusion in spatially inhomogeneous systems

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Plan of talk

1. Coarse graining effective diffusion coefficients

2. Single file diffusion

3. Single file diffusion in terms of effusion

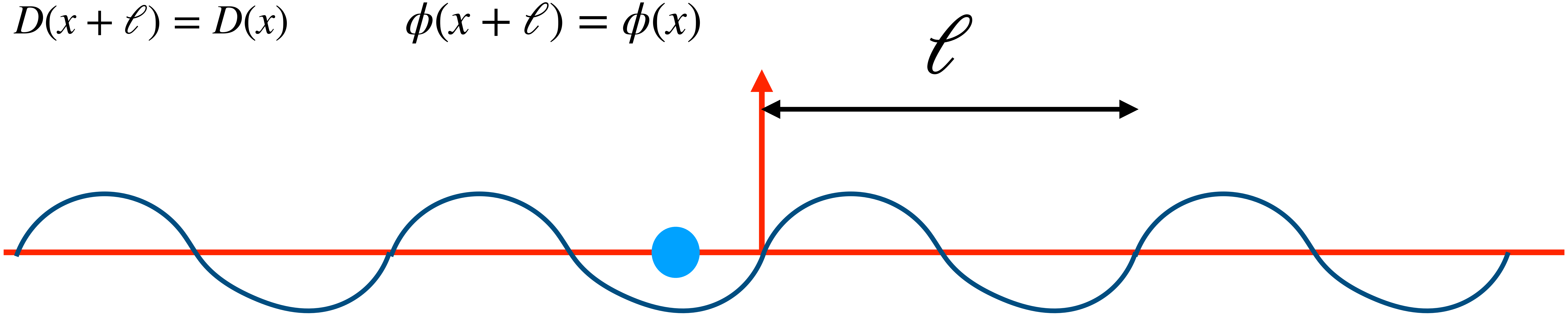
4. Treatment using physics take on homogenisation theory from mathematics

Coarse graining for single particle

Fokker-Planck equation $$\frac{\partial p(x,t)}{\partial t} = \hat{H}p(x,t), \qquad \hat{H} \equiv \frac{\partial}{\partial x}\left[D(x)\left(\beta\frac{d\phi(x)}{dx} + \frac{\partial}{\partial x}\right)\right]$$

Single particle in 1d with spatially varying periodic local diffusivity and potential

$$D(x+\ell) = D(x) \qquad \phi(x+\ell) = \phi(x)$$



Expect that at late times $$\langle [X(t) - X(0)]^2 \rangle \simeq 2D_{\text{eff}}t$$ **(No drift or bias in periodic system)**

D_{eff} **Effective (late time)diffusion constant**

Effective coarse grained equation

Assume that on large length and time scales

$$\frac{\partial p(x,t)}{\partial t} = \hat{H}_{\text{eff}}\, p(x,t), \qquad \hat{H}_{\text{eff}} \equiv D_{\text{eff}} \frac{\partial^2}{\partial x^2}$$

Lifson-Jackson J. Chem. Phys. 36, 2410 (1962) - solve mean first passage time to some large distance $L \gg \ell$ for both problems and compare (can be done analytically in 1 d)

$T(x)$ **Mean first passage time to $\pm L$ starting from x**

$$\hat{H}^\dagger T(x) = -1 \qquad T(L) = T(-L) = 0$$

$$D_{\text{eff}} = \frac{\ell^2}{\left[\int_0^\ell dx e^{\beta\phi(x)}/D(x)\right]\left[\int_0^\ell dx e^{-\beta\phi(x)}\right]}$$

Effective diffusion constant can be evaluated directly from definition $\langle [X(t) - X(0)]^2 \rangle \simeq 2D_{\rm eff} t$

H. Brenner and D.A. Edwards, Macrotransport processes, 1993

G. A. Pavliotis and A. Stuart, Multiscale Methods: Averaging and Homogenization, 2008

T. Guérin and D.S. Dean, Phys. Rev. Lett. 15, 020601 (2015) - Kubo formulas

$$\frac{\partial p}{\partial t} = -Hp \qquad Hf = -\frac{\partial}{\partial x_i}\left(\frac{\partial}{\partial x_j}(\kappa_{ij}(\mathbf{x})f(\mathbf{x})) - A_i(\mathbf{x})f(\mathbf{x})\right)$$

$$P_s(\mathbf{x}) \qquad J_{si}(\mathbf{x}) = -\frac{\partial}{\partial x_j}(\kappa_{ij}(\mathbf{x})P_s(\mathbf{x})) + A_i(\mathbf{x})P_s(\mathbf{x})$$

Steady state density and current on periodic unit cell Ω

$$Hf_i(\mathbf{x}) = \left[\left(A_i(\mathbf{x}) - \int_\Omega d\mathbf{y} A_i(\mathbf{y})P_s(\mathbf{y})\right)P_s(\mathbf{x}) - 2\frac{\partial}{\partial x_j}(\kappa_{ij}(\mathbf{x})P_s(\mathbf{x}))\right]$$

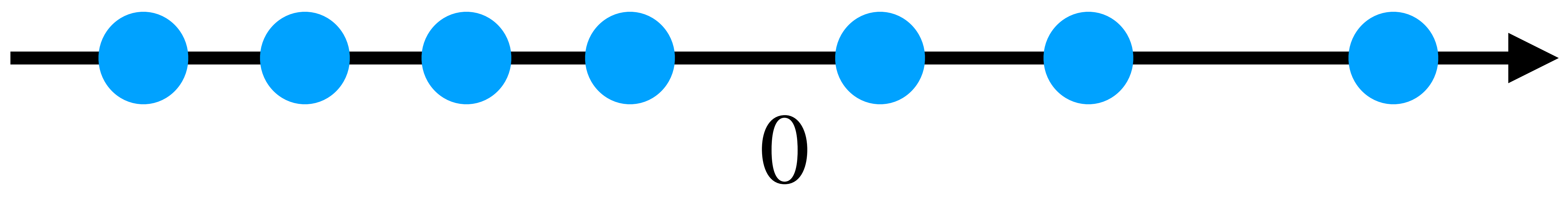
Auxillary function

$$\int_\Omega d\mathbf{x}\ f_i(\mathbf{x}) = 0$$

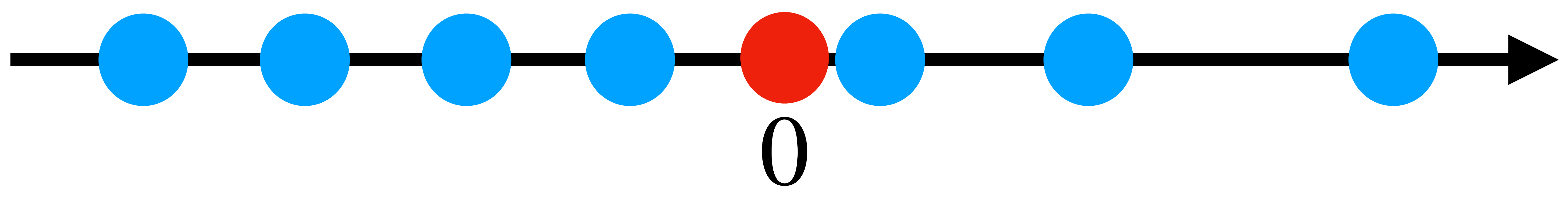
Orthogonality condition

$$D_{ii} = \int_\Omega d\mathbf{x}\ \kappa_{ii}(\mathbf{x})P_s(\mathbf{x}) + \int_\Omega d\mathbf{x} A_i(\mathbf{x})f_i(\mathbf{x}).$$

Single file diffusion



Brownian particles with hard-core interactions in a homogeneous system
- reflecting boundary conditions



Y_t **position of tracer particle (identical to others) started at** 0 **at** $t = 0$

Tracer dispersion

Average over Brownian motion (thermal noise) $\langle \cdots \rangle$

Average over uniform (ideal gas) initial conditions with density $\bar{\rho}$, $\overline{\cdots}$

S. Alexander and P. Pincus, Phys. Rev. B 18 2011 (1978)
T. Harris, J. Appl. Probab. 2, 323 (1965)
P.L. Krapivsky, K. Mallick and T. Sadhu, Phys. Rev. Lett. 113 078101 (2014).

Annealed average

$$\langle Y^2(t)\rangle_{\rm ac} = \overline{\langle Y^2(t)\rangle} - \overline{\langle Y(t)\rangle}\ \overline{\langle Y(t)\rangle} = \frac{2}{\bar{\rho}}\sqrt{\frac{Dt}{\pi}}$$

Quenched average

$$\langle Y^2(t)\rangle_{\rm qc} = \overline{\langle Y^2(t)\rangle} - \overline{\langle Y(t)\rangle\ \langle Y(t)\rangle} = \frac{\sqrt{2}}{\bar{\rho}}\sqrt{\frac{Dt}{\pi}}$$

Quenched average here is mathematically identical to result for regularly spaced initial conditions (more generally hyper uniform initial conditions)

Simple question

In periodic inhomogeneous systems is the following true

$$\langle Y^2(t)\rangle_{\mathrm{ac}} = \frac{2}{\bar{\rho}}\sqrt{\frac{D_{\mathrm{eff}}t}{\pi}}$$

$$\langle Y^2(t)\rangle_{\mathrm{qc}} = \frac{\sqrt{2}}{\bar{\rho}}\sqrt{\frac{D_{\mathrm{eff}}t}{\pi}}$$

Numerical simulations of SFD systems with periodic potentials say yes (varying diffusivity not considered).

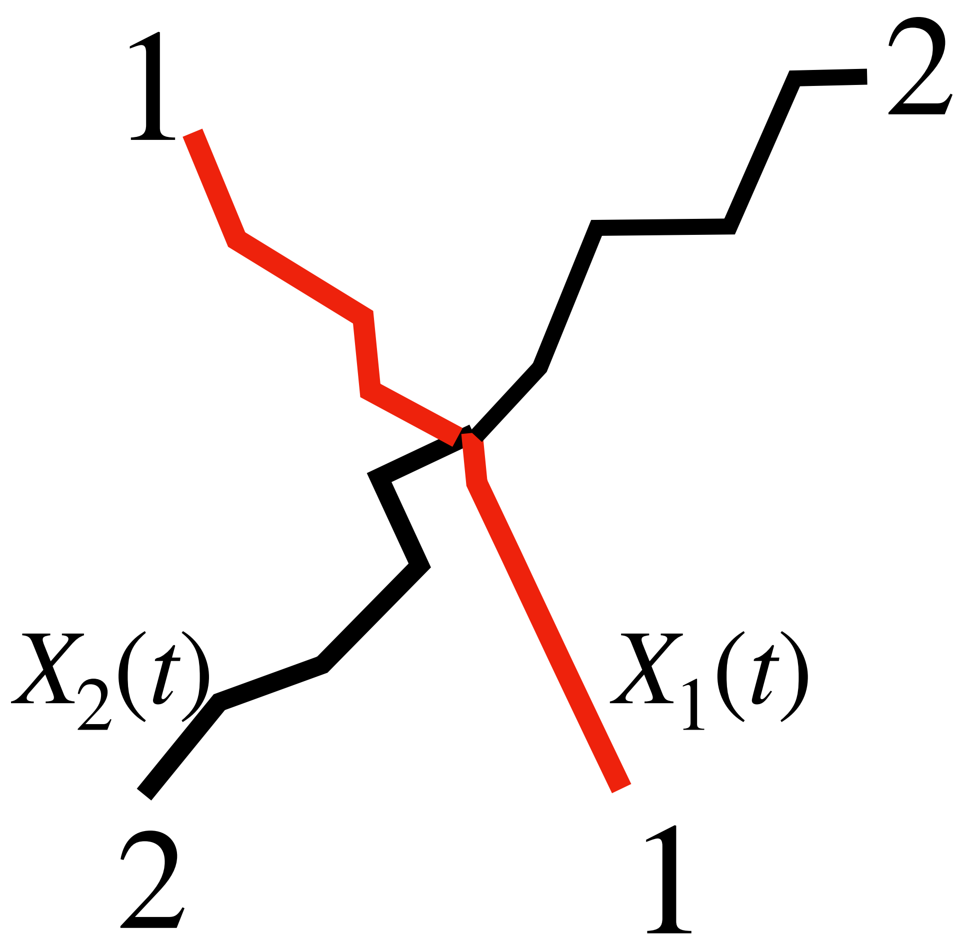
A. Taloni and F. Marchesoni, Phys. Rev. Lett. 96, 020601 (2006).
D. Lips, A. Ryabov, and P. Maass, Phys. Rev. E 100, 052121 (2019).

Physically it is difficult to see how it could not be true - but let's prove it

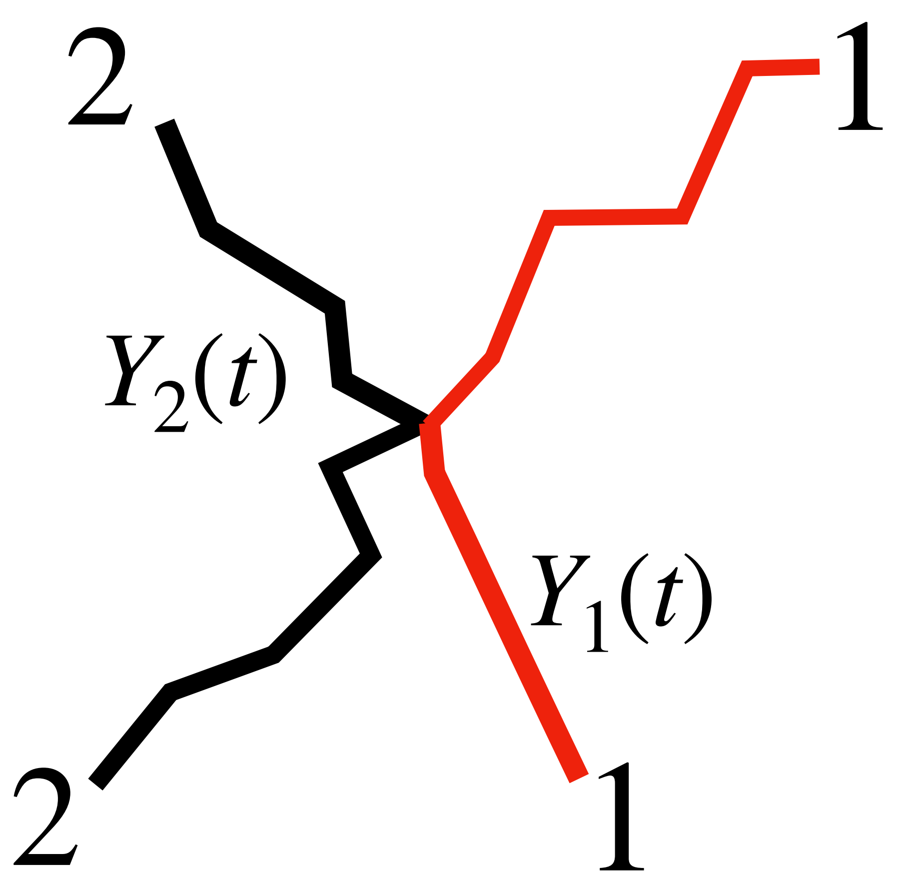
SFD and free particles

T. E. Harris, J. Appl. Probab. 2, 323 (1965)

Elastically colliding stochastic processes
articles do not interact but change labels when they cross



Non-interacting processes



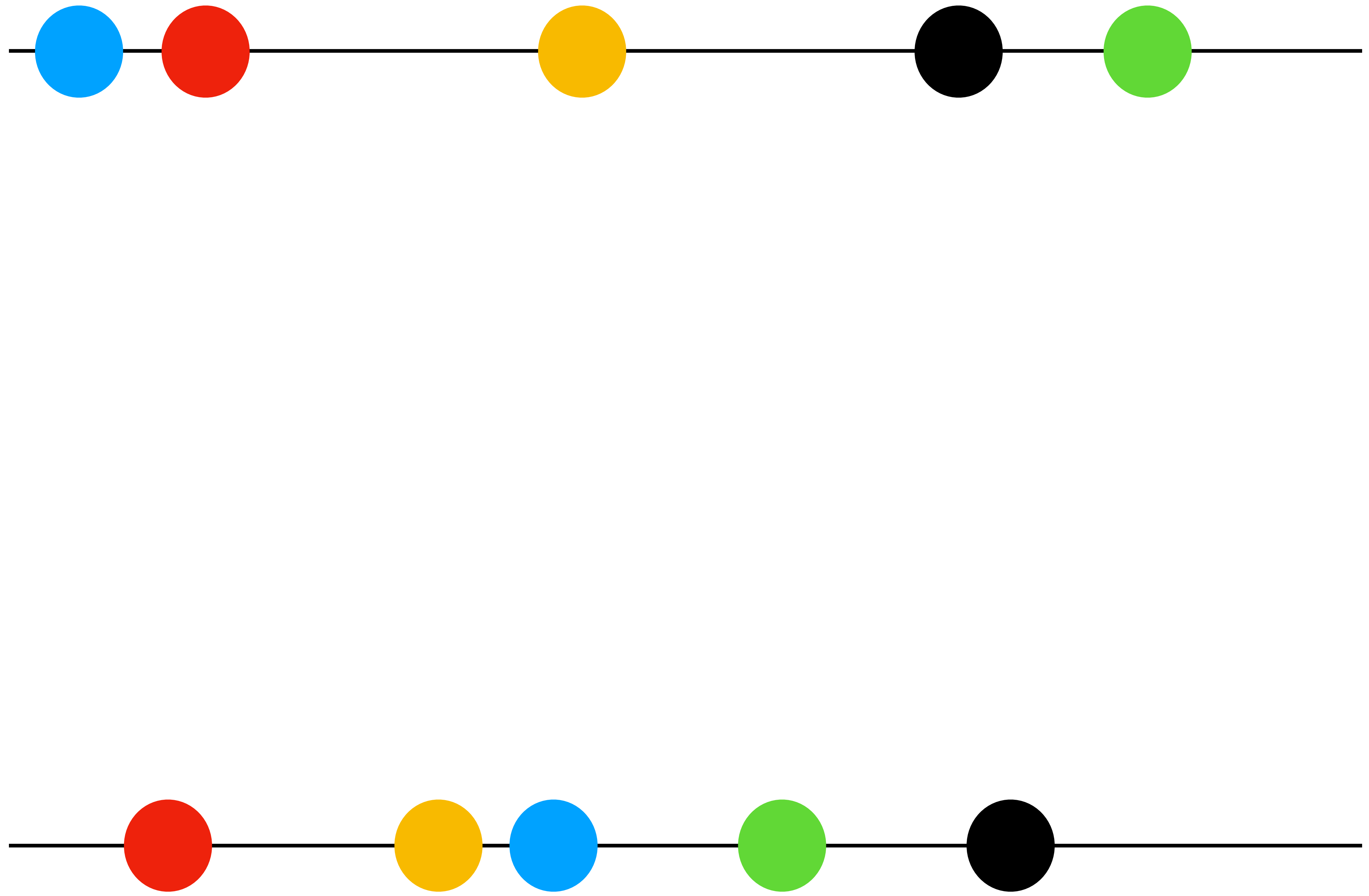
Elastically colliding processes
ECP

$$Y_1(t) = \max(X_1(t), X_2(t))$$

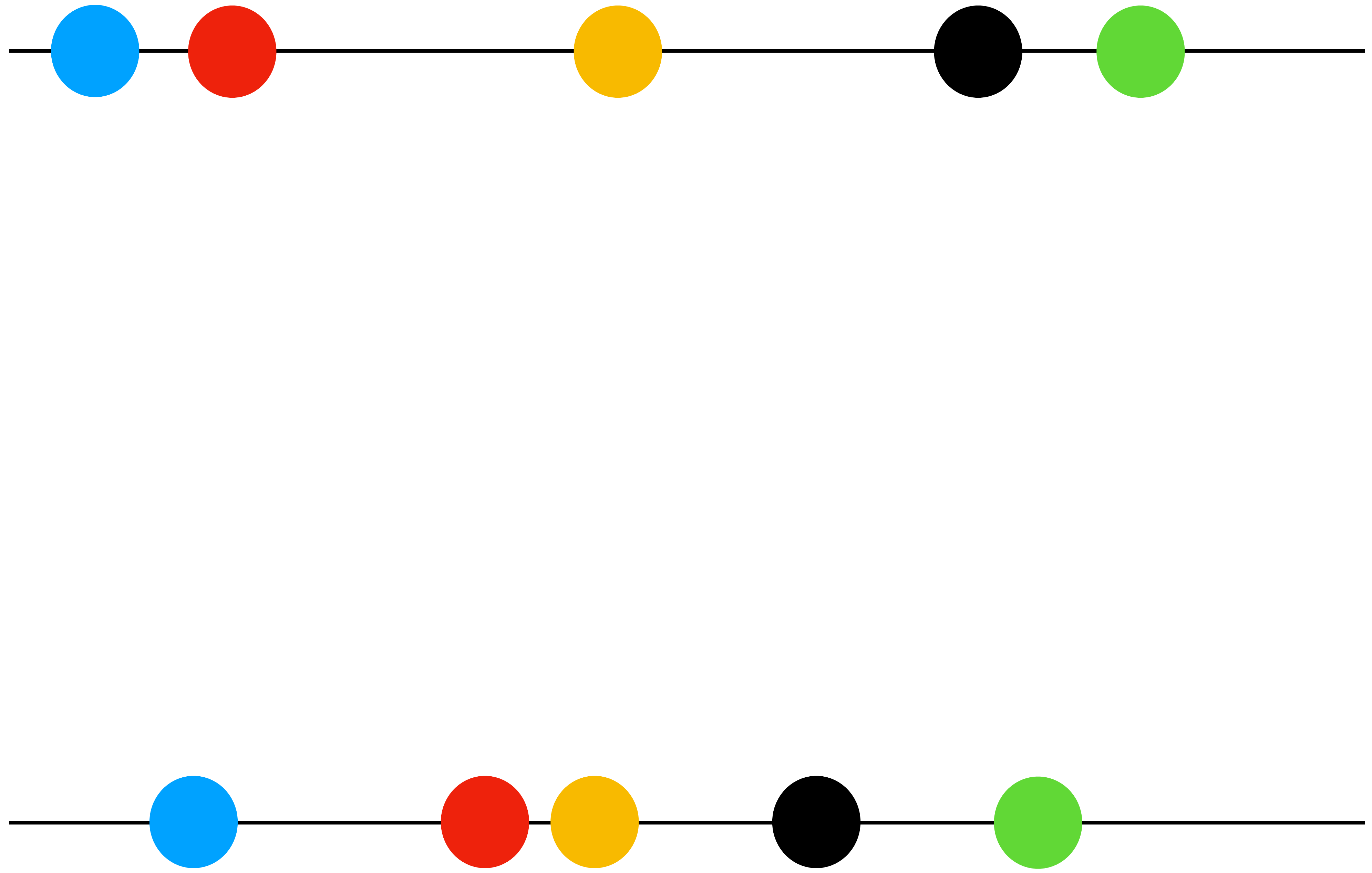
$$Y_2(t) = \min(X_1(t), X_2(t))$$

No interaction seen
if particle numbers are
not observed (not a SEP)

Without relabelling



With relabelling



Keeping track of the tracer

Free particle density $\rho(x) = \sum_i \delta(X_i(t) - x)$

Tracer particle position $Y(t),\ Y(0) = 0$

$$\int_{-L}^{0} dx\ \rho(x,0) = \int_{-L}^{Y(t)} dx\ \rho(x,t)$$

Number of particles to left of tracer under relabelling is constant

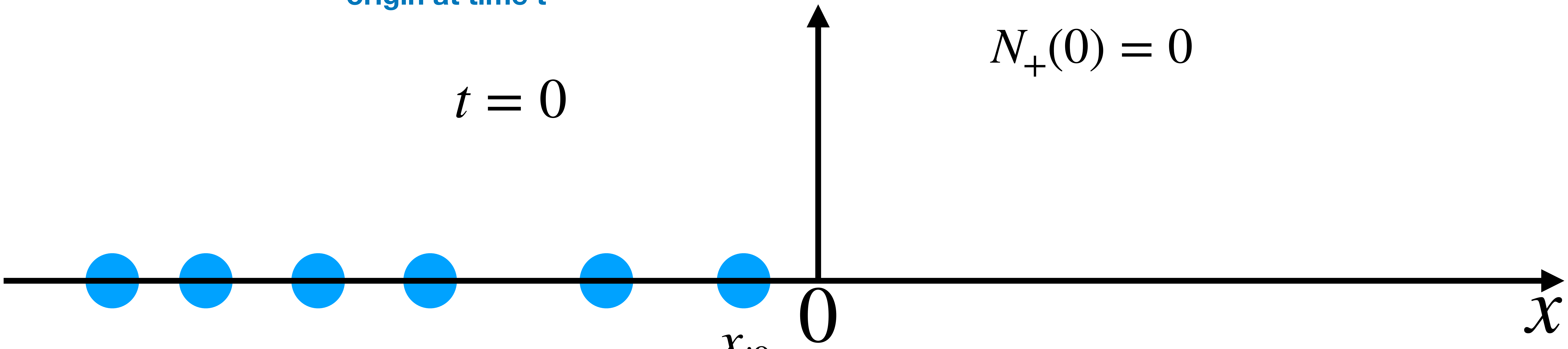
$$\int_{0}^{Y(t)} dx\ \rho(x,0) = \int_{-L}^{0} dx\ \rho(x,0) - \rho(x,t)$$

General effusion problem

$N_+(t)$ Number of particles to right of origin at time t

$t = 0$

$N_+(0) = 0$



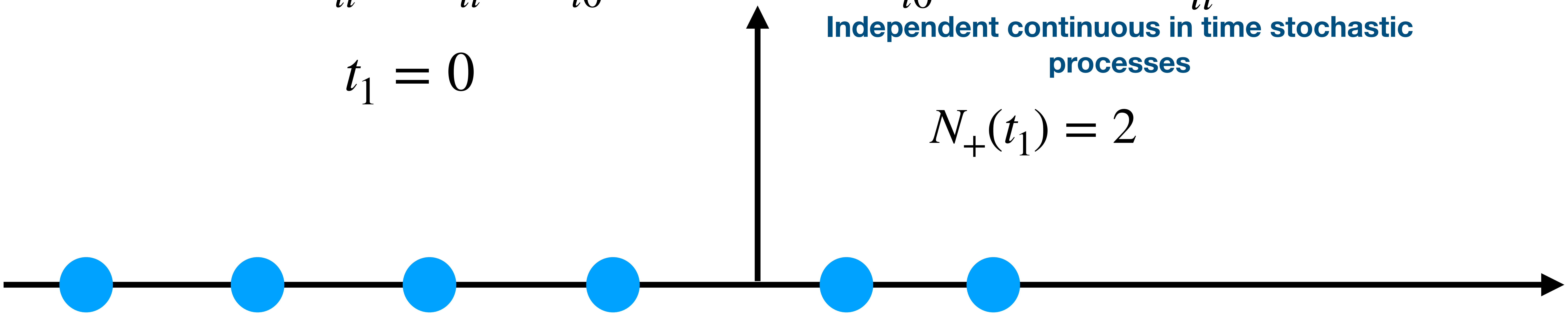
$X_{it} = Y_{it} + x_{i0}$

$Y_{i0} = 0$ Y_{it}

Independent continuous in time stochastic processes

$t_1 = 0$

$N_+(t_1) = 2$

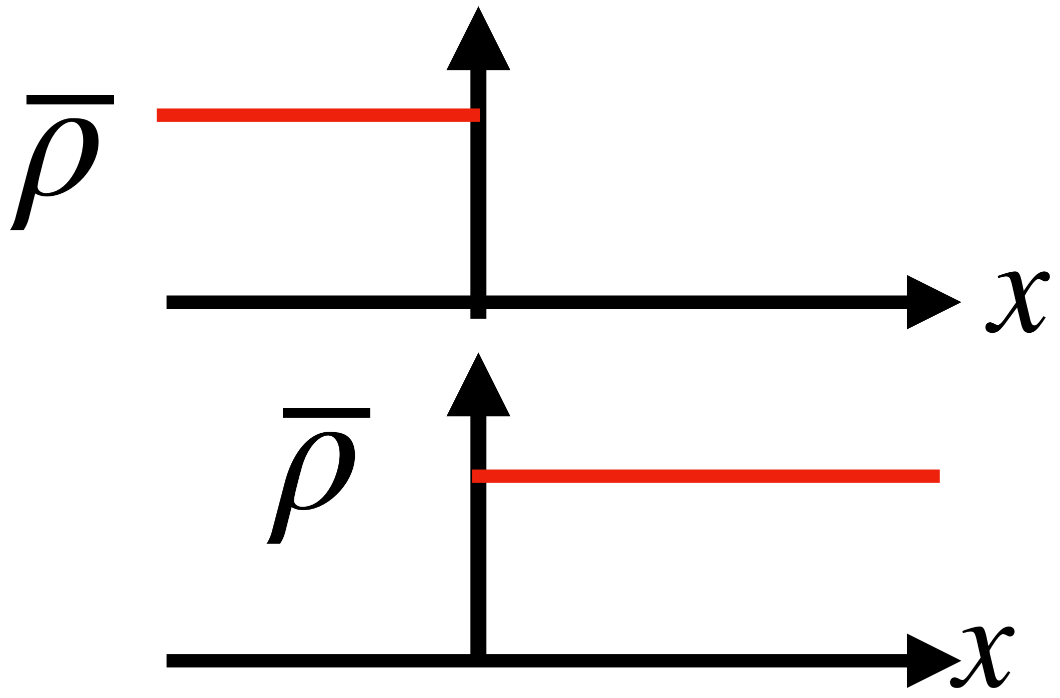


Links with two independent effusion problems

$$\rho(x,t) = \rho_R(x,t) + \rho_L(x,t)$$

density due to particles initially right of 0 (→ ρ_R)

density due to particles initially left of 0 (→ ρ_L)



$$N_+(t) = \int_0^\infty dx\ \rho_{\rm L}(x,t)$$

$$N_-(t) = \int_0^\infty dx\ \rho_{\rm R}(x,t)$$

Two independent effusion problems

$$\int_0^{Y(t)} dx\ \rho(x,t) = N_+(t) - N_-(t)$$

Key result

$$Y(t) \simeq \frac{1}{\bar{\rho}}\left[N_+(t) - N_-(t)\right]$$

Assuming $|Y(t)| \to \infty$ as $t \to \infty$ central limit theorem

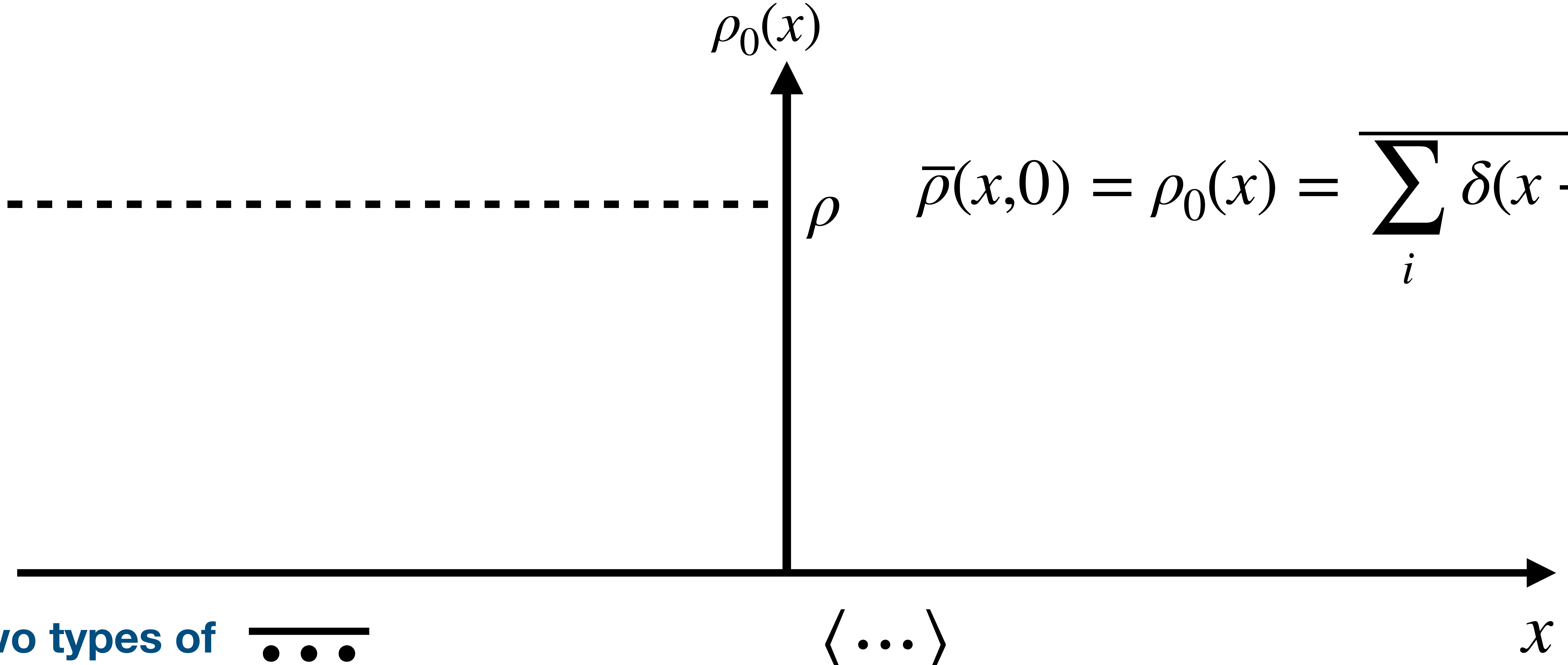
D. Durr, S. Goldstein, and J. L. Lebowitz, Commun. Pure Appl. Math. 38, 573 (1985)

$$\langle Y^2(t)\rangle_{\rm a/qc} \simeq \frac{1}{\bar{\rho}^2}\langle\left[N_+(t) - N_-(t)\right]^2\rangle_{a/qc}$$

Coarse grained picture -step like initial density profile

B. Derrida and A. Gerschenfeld, J. Stat. Phys. 137, 978 (2009) - macroscopic fluctuation theory (BM)

Banerjee, S. N. Majumdar, A. Rosso, and G. Schehr, Phys. Rev. E 101, 052101 (2020) - direct calculation



$$\bar{\rho}(x,0) = \rho_0(x) = \overline{\sum_i \delta(x - x_{i0})}$$

Two types of averaging $\overline{\cdots}$ $\langle \cdots \rangle$

initial conditions x_{i0} stochastic trajectories Y_{it}

$$\langle Q^2 \rangle_{ac} = \overline{\langle Q^2 \rangle} - \overline{\langle Q \rangle}^2$$

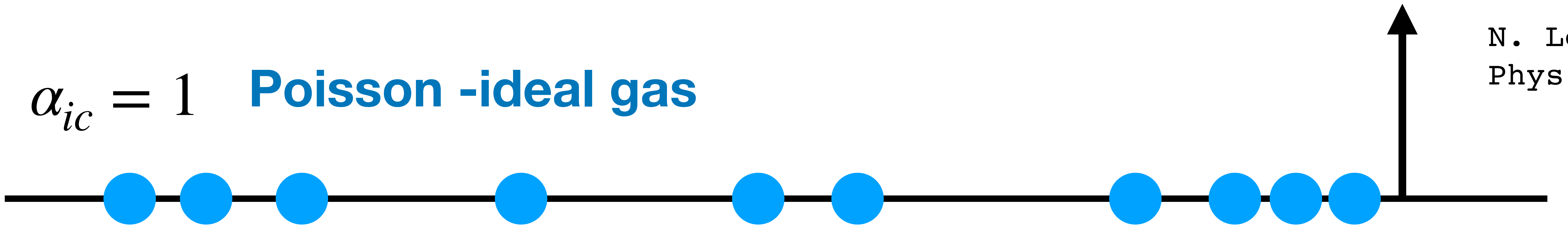
$$\langle Q^2 \rangle_{qc} = \overline{\langle Q^2 \rangle} - \overline{\langle Q \rangle^2}$$

Role of initial conditions

T. Banerjee, R. L. Jack, and M. E. Cates
Phys. Rev. E 106, (2022),

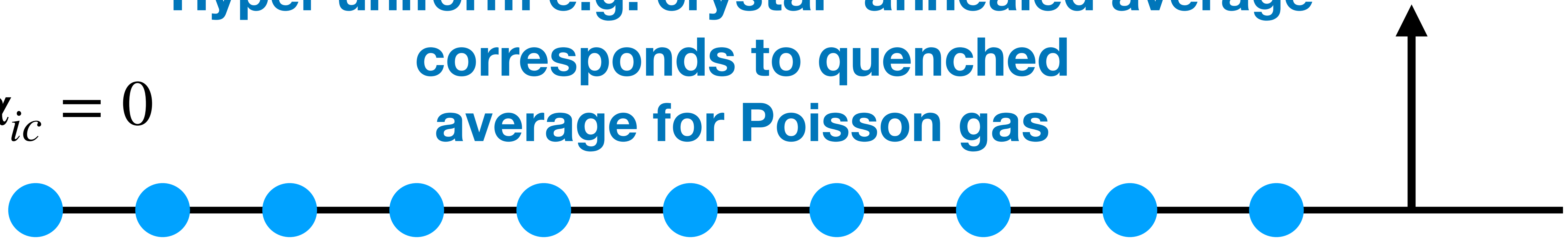
N. Leibovich and E. Barkai,
Phys. Rev. E 88, 032107 (2013)

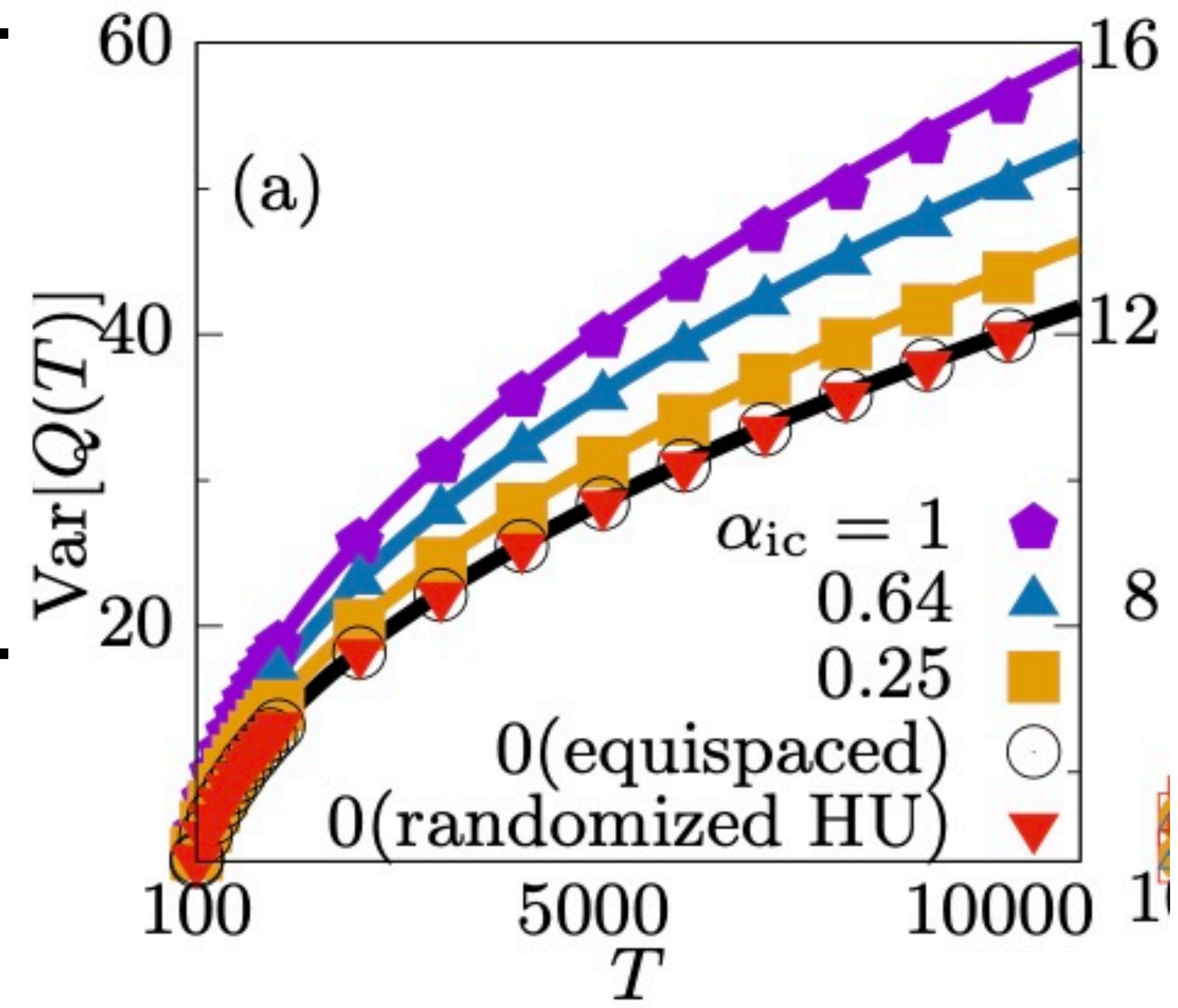
$\alpha_{ic} = 1$ **Poisson -ideal gas**



Hyper uniform e.g. crystal -annealed average corresponds to quenched average for Poisson gas

$\alpha_{ic} = 0$





$\overline{\langle N^2_{\mathbb{R}^+}(t)\rangle} - \overline{\langle N_{\mathbb{R}^+}(t)\rangle}^2$ **depends at all times on initial conditions via**

Fano-factor
Generalised compressibility

$$\alpha_{ic} = \lim_{\ell\to\infty} \frac{\mathrm{Var}\ n(\ell)}{\overline{n(\ell)}} = \lim_{q\to 0} S(q)$$

Structure factor

General solution to effusion problem

D.S.D, S.N. Majumdar and G. Schehr, J.Stat. Mech.063208 (2023).

$\overline{\rho_{\mathrm{L}}(x)} = (\ell_0 M/L)P_0(x)$ **initial density to left of origin $x \in [-L,0]$ of period ℓ_0** $\bar{\rho} = M/L$

ℓ_0 doesn't have to be the same as ℓ

$$\overline{\langle N_+(t)\rangle} = \int_{-\infty}^{0} \overline{\rho_L(x_0)} \int_0^\infty dx p(x,t\,|\,x_0,0)$$ **average**

$$\langle N_+^2(t)\rangle_{\mathrm{ac}} = \int_{-\infty}^{0} dx_0 \overline{\rho_{\mathrm{L}}(x_0)} \int_0^\infty dx p(x,t\,|\,x_0,0) = \overline{\langle N_+(t)\rangle}$$ **annealed variance same as average - Poisson**

$$\langle N_+^2(t)\rangle_{\mathrm{qc}} = \int_{-\infty}^{0} dx_0 \overline{\rho_{\mathrm{L}}(x_0)} \int_0^\infty dx p(x,t\,|\,x_0,0) - \int_{-\infty}^{0} dx_0 \overline{\rho_{\mathrm{L}}(x_0)} \int_0^\infty dx p(x,t\,|\,x_0,0) \int_0^\infty dx' p(x',t\,|\,x_0,0)$$

quenched variance

$$\frac{\partial p(x,t\,|\,x_0)}{\partial t} = \hat{H}p(x,t\,|\,x_0), \qquad \hat{H} \equiv \frac{\partial}{\partial x}\left[D(x)\left(\beta\frac{d\phi(x)}{dx} + \frac{\partial}{\partial x}\right)\right]$$

$p(x,t\,|\,x_0)$ propagator for FP equation

Solve in terms of initial coordinate

$$\frac{f(x_0, t)}{P_B(x_0)} = \int_{-\infty}^{\infty} dx\ p(x, t \mid x_0, 0)\Theta(x)$$

$$P_B(x) = Z^{-1} e^{-\beta\phi(x)}$$

Boltzmann distribution over one period ℓ

$$\langle N_+^2(t)\rangle_{ac} = \bar{\rho}\ell_0 \int_{-\infty}^{\infty} dx_0 \Theta(-x_0) P_0(x_0) \frac{f(x_0, t)}{P_B(x_0)}$$

$$\frac{\partial f(x, t)}{\partial t} = \hat{H} f(x, t)$$

Obeys forward FP equation

$$f(x, 0) = \Theta(x) P_B(x)$$

Initial conditions

$$\hat{H}\tilde{f}(x, s) = s\tilde{f}(x, s) - f(x, 0)$$

Laplace transform

Homogenisation à la physicist

$$\tilde{f}(x,s) = \frac{1}{s}\sum_{n=0}^{\infty} s^{\frac{n}{2}} F_n(x, \sqrt{s}x)$$

$F_n(x,y)$ **Periodic in x with period ℓ - fast variable**

$$(\partial/\partial x) \to (\partial/\partial x) + s^{1/2} \cdot (\partial/\partial y)$$

Perturbatively solve for small s (corresponding to large t)

systematic separation of variable $F_n(x,y) = M_n(x)K_n(y)$

$$F_0(x,y) = P_\mathrm{B}(x)K_0(y)$$

Order s^{-1}

$$\frac{\partial}{\partial x}\left[D(x)\left(\beta\frac{d\phi(x)}{dx}F_1(x,y) + \frac{\partial F_1(x,y)}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[D(x)\left(\beta\frac{d\phi(x)}{dx}F_0(x,y) + \frac{\partial F_0(x,y)}{\partial x}\right)\right] + \frac{\partial}{\partial x}\left[D(x)\frac{\partial F_0(x,y)}{\partial y}\right] = 0$$

Order $s^{-\frac{1}{2}}$

$$\frac{\partial}{\partial x}\left[D(x)\left(\beta\frac{d\phi(x)}{dx}F_2(x,y) + \frac{\partial F_2(x,y)}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[D(x)\left(\beta\frac{d\phi(x)}{dx}F_1(x,y) + \frac{\partial F_1(x,y)}{\partial x}\right)\right] + \frac{\partial}{\partial x}\left[D(x)\frac{\partial F_1(x,y)}{\partial y}\right] + D(x)\frac{\partial^2 F_0(x,y)}{\partial y^2} = F_0(x,y) - \Theta(y)P_0(x)\,.$$

Order 1

Effective or coarse grained diffusion equation

$$D_{\text{eff}} \frac{\partial^2 K_0(y)}{\partial y^2} = K_0(y) - \Theta(y)$$

D_{eff}- Lifson-Jackson result !

$$\widetilde{\langle N_+^2 \rangle}_{\text{ac}} = \frac{\bar{\rho}\ell_0}{2s} \int_{-\infty}^{0} dx_0 \; P_0(x_0) \exp\left(\sqrt{\frac{s}{D_{\text{eff}}}} x_0 \right).$$

$$P_0(x) = \frac{1}{\ell_0} \left[1 + \sum_{n \neq 0} \exp\left(\frac{2\pi i n x}{\ell_0} \right) \int_0^{\ell} dx' P_0(x') \exp\left(-\frac{2\pi i n x'}{\ell_0} \right) \right]$$

Fourier series

$$\int_{-\infty}^{0} dx_0 \exp\left(\sqrt{\frac{s}{D_{\text{eff}}}} x_0 + i k_n x_0 \right) = \frac{1}{i k_n + \sqrt{s/D_{\text{eff}}}}$$

Mode n= 0 dominates at late times

dependence on $P_0(x)$ goes away

Leading order late time result

$$\langle N_+^2(t) \rangle_{\text{ac}} = \bar{\rho} \sqrt{\frac{D_{\text{eff}} t}{\pi}}$$

agrees with intuition

Simulation results- potential

$$\beta\phi(x) = E[1 - \cos(2\pi x/\ell)]$$

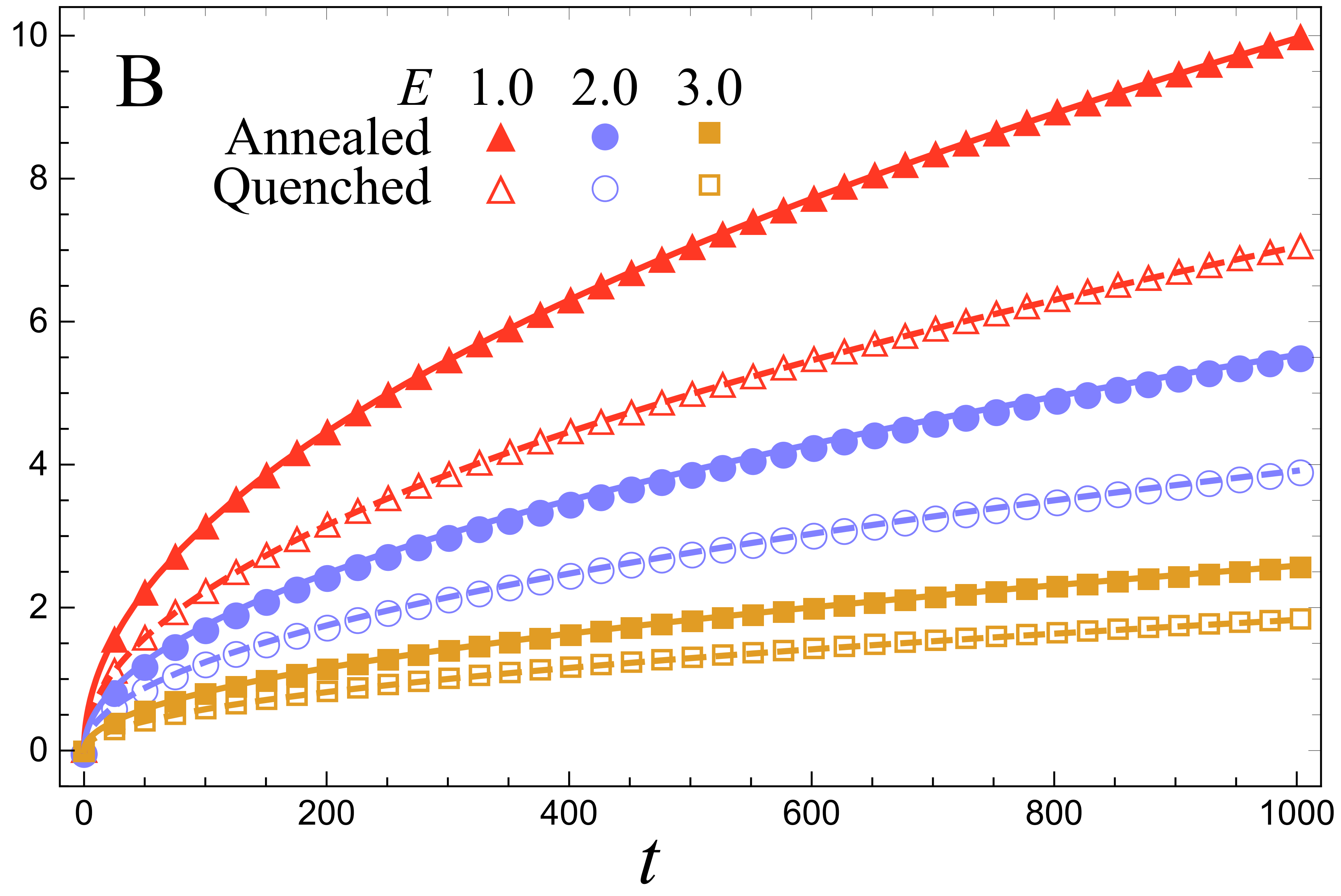
A. Taloni and F. Marchesoni, Phys. Rev. Lett. 96, 020601 (2006).
D. Lips, A. Ryabov, and P. Maass, Phys. Rev. E 100, 052121 (2019).

$$D(x) = D_0$$

Theoretical predictions

$$\langle Y^2(t; E, \bar{\rho})\rangle_{\mathrm{ac}} = \frac{2}{\bar{\rho} I_0(E)}\sqrt{\frac{D_0 t}{\pi}} \qquad \langle Y^2(t; E, \bar{\rho})\rangle_{\mathrm{qc}} = \frac{\sqrt{2}}{\bar{\rho} I_0(E)}\sqrt{\frac{D_0 t}{\pi}}$$

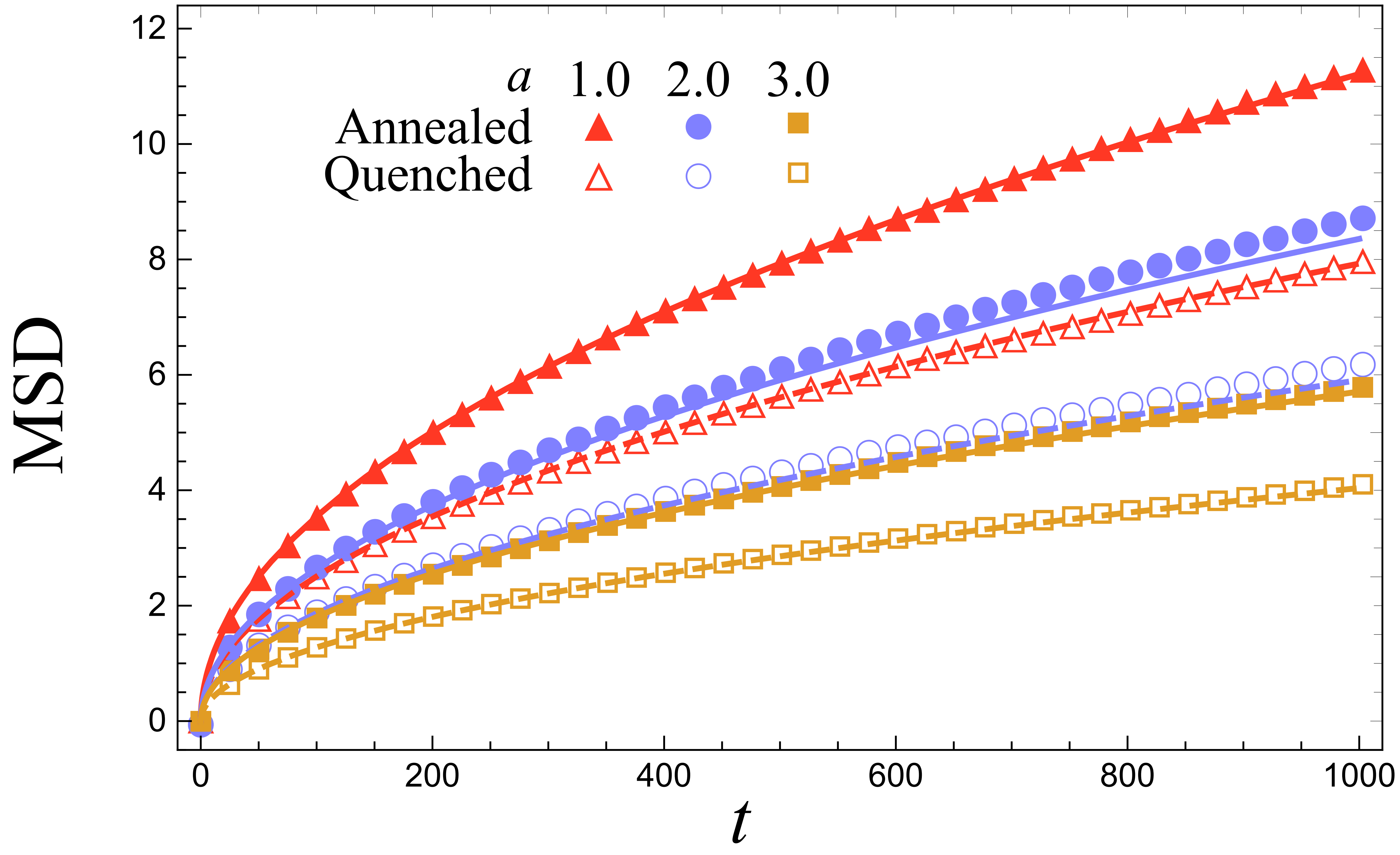
$I_0(z)$ **modified Bessel function**



Simulations-diffusivity

$$D(x) = D_0 \exp[a\cos(2\pi x/\ell)] \qquad \phi = 0$$

$$\langle Y^2(t; a, \bar{\rho})\rangle_{\mathrm{ac}} = \frac{2}{\bar{\rho}}\sqrt{\frac{D_0 t}{I_0(a)\pi}} = F_{\mathrm{eff}}\sqrt{t} \qquad \langle Y^2(t; a, \bar{\rho})\rangle_{\mathrm{qc}} = \frac{\sqrt{2}}{\bar{\rho}}\sqrt{\frac{D_0 t}{I_0(a)\pi}} = F_{\mathrm{eff}}\sqrt{t}$$



Conclusion

Long time effective diffusion constant can be used to characterise the long time SFD behavior

A form of homogenisation theory from applied mathematics can be adapted to prove the result

It would be interesting to see if homogenisation theory can be applied to other problems in statistical physics - for example to justify macroscopic fluctuation theory

L. Bertini, A. De Sole, D. Gabrielli, G. Jona-Lasinio and C. Landim,
Phys. Rev. Lett. 87, 040601 (2001)