

FIG. 5: Motion of tagged particle in a box is shown for $N = 1, 10, 70$. Simulation results (squares) are taken from [25] (see text). At short time simulations exhibit normal diffusion $\langle (x_T)^2 \rangle = 2Dt$ as illustrated by the straight dashed line which is a guide to the eye. Our theory is expected to work well in the large N limit and when many collision events between tagged particle and surrounding Brownian particles took place. Hence agreement between theory (solid line) and simulation is reasonable at most only for $N = 70$ and not for too short times.

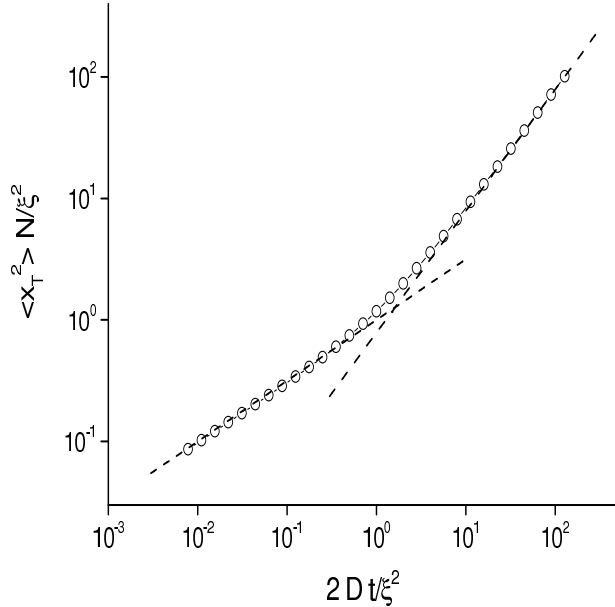


FIG. 6: Scaled mean square displacement of the tagged particle with Gaussian initial conditions of the packet of particles exhibits a transition between short time $\langle (x_T)^2 \rangle \propto t^{1/2}$ law to $\langle (x_T)^2 \rangle \propto t$ behavior. Dashed lines are short and long time asymptotic behavior Eq. (60), circles represent Eq. (59).

Changing variables according to $y^2/2 = (x - x_0)^2/4Dt$ and using dimensionless parameter $\xi = \xi/\sqrt{2Dt}$, we find

$$\mathcal{R} = \frac{1}{2} + \frac{1}{\xi} \sqrt{\frac{2}{\pi}} \int_0^\infty d\tilde{x}_0 e^{-\frac{(\tilde{x}_0)^2}{2\xi^2}} \frac{\text{Erf}(\tilde{x}_0/\sqrt{2})}{2} \quad (56)$$

where $\text{Erf}(\tilde{x}_0/\sqrt{2})/2 = \int_0^{\tilde{x}_0} e^{-y^2/2} dy/\sqrt{2\pi}$ is the error function [42]. Mathematica solves the integral in Eq. (56) and we find

$$\mathcal{R} = \frac{1}{2} + \frac{1}{\pi} \text{arccot} \left(\frac{\sqrt{2Dt}}{\xi} \right). \quad (57)$$

For short times $\sqrt{Dt} \ll \xi$ we have $\mathcal{R} \sim 1 - \frac{\sqrt{2Dt}}{\pi\xi}$, namely most particles did not have time to cross the origin, while in the opposite limit $\lim_{t \rightarrow \infty} \mathcal{R} = 1/2$ due to the symmetry of initial conditions. The calculation of r Eq. (34) using Eqs. (23,54) is straightforward

$$r = \frac{1}{2\sqrt{\pi Dt} \sqrt{1 + \xi^2/2Dt}}, \quad (58)$$

Inserting Eqs. (57,58) in Eq. (37) we find

$$\langle (x_T)^2 \rangle \sim \xi^2 \frac{\pi}{N} \left(1 + \frac{2Dt}{\xi^2} \right) \left[\frac{1}{4} - \frac{1}{\pi^2} \text{arccot}^2 \left(\sqrt{\frac{2Dt}{\xi^2}} \right) \right], \quad (59)$$

This solution is shown in Fig. 6 with its two limiting behaviors

$$\langle (x_T)^2 \rangle \sim \begin{cases} \xi \frac{\sqrt{2Dt}}{N} & \text{short times } 2Dt \ll \xi^2 \\ \frac{\pi D}{2N} t & \text{long times } 2Dt \gg \xi^2. \end{cases} \quad (60)$$

For short times the particles do not have time to disperse; hence, the motion of the tagged particle is slower than normal, increasing as $t^{1/2}$ which is similar to the single file diffusion with a uniform density Eq. (50). Roughly speaking, for short times the tagged particle sees a uniform density of particles with $\rho = N/\xi$. For long times we recover the behavior in Eq. (27) since the scale of diffusion is much larger than ξ . Hence if we start with a Gaussian or delta function packet we get in the long time limit similar behavior, as we showed.

C. Particles in Harmonic Oscillator

Consider particles in a harmonic potential $V(x) = m\omega^2 x^2/2$ where $\omega > 0$ is the harmonic frequency. The single particle undergoes an Ornstein Uhlenbeck process [38] and the corresponding single particle Green function is

$$g(x, x_0, t) =$$

$$\frac{1}{\sqrt{2\pi D\tau} (1 - e^{-2t/\tau})} \exp \left[-\frac{(x - x_0 e^{-t/\tau})^2}{2D\tau (1 - e^{-2t/\tau})} \right], \quad (61)$$