What model describes a Brownian particle?

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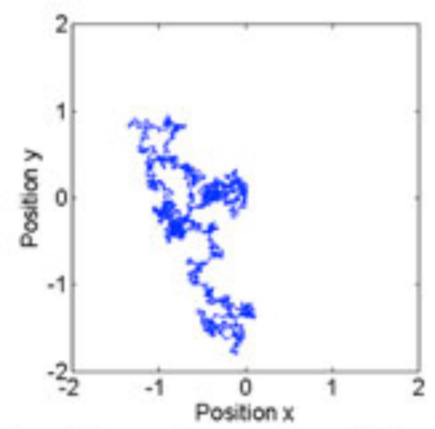
Introduction

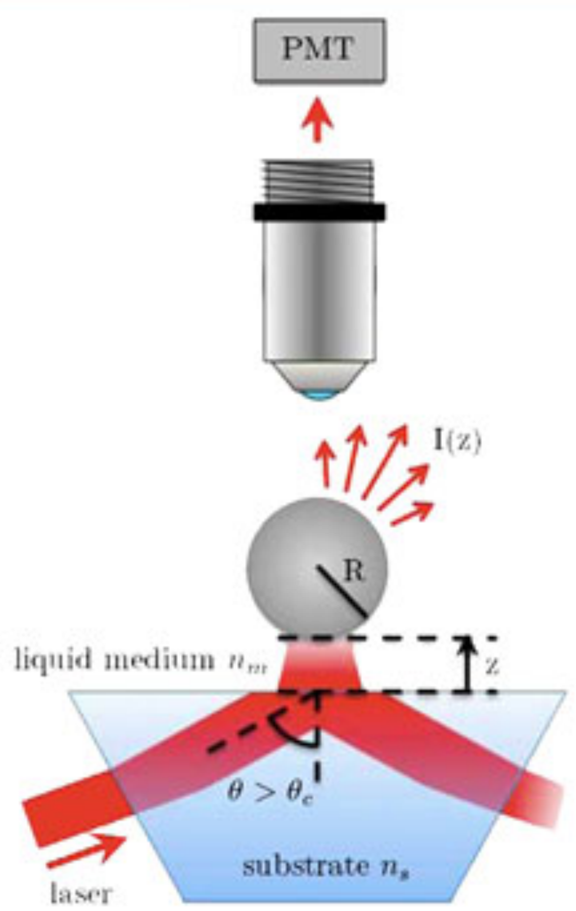
An example of a Brownian particle is a small colloidal particle in water. The particle is big enough to measure movements, but small enough that collisions between the particle and water molecules cause irregular motion. The presence of thermal noise prevents us from using deterministic equations of motion for microscopic objects. How do we mathematically describe a Brownian particle with a small mass and experiencing hydrodynamic effects in friction and noise? The dynamics of Brownian motion have many applications in biology, physics, chemistry and economics.



A simulation of two-dimensional Brownian motion.
Example: A pollen particle in a petri dish far away from walls.

Experiment

This work was motivated by an experiment [1] where a colloidal particle (micrometer in diameter) in water was held near a wall using an optical trap. The average forces in the vertical direction were then measured. The results were not as expected because of an extra force term arising from the thermal noise.



Experimental apparatus set up by [1]. The particle is close to the barrier causing hydrodynamic effects in the friction and noise terms

Model

To model the experiment, we use stochastic differential equations (SDE). For a particle of mass m, force F(x), the position $x^m(t)$ is given by the Newton equation,

$$m\frac{d^2x^m(t)}{dt^2} = \underbrace{F(x^m(t)) - \frac{k_BT}{D(x^m(t))}\frac{dx^m(t)}{dt}}_{\text{deterministic forces}} + \underbrace{\frac{k_BT\sqrt{2}}{\sqrt{D(x^m(t))}}\eta(t)}_{\text{random}}$$

where the friction and random forces depend on a hydrodynamic diffusion coeffecient D(x), that depends on the distance of the particle from the wall. We approximate the dynamics by assuming the random force is an uncorrelated mean-zero Gaussian process and the friction effects dominate the inertia. Mathematically, we take the limit as mass $m \to 0$. The expected limit,

$$x(t) = x(0) + \int_0^t \frac{F(x(t))D(x(t))}{k_BT}\,dt + \int_0^t \sqrt{2D(x(t))}\,dW(t)$$

is called the Smoluchowski-Kramers approximation.

Methods

To study the dynamics as $m \to 0$, we use a powerful connection between stochastic differential equations and partial differential equations. The following outlines the strategy of for deriving the small mass limit:

1) the position $x^m(t)$, has a probability density function, $p_m(x,v)$, that satisfies the Backward-Kolomogorov partial differential equation.

$$p_m(x,v) = p_0(x) + \sqrt{m}\,p_1(x,v) + m\,p_2(x,v) + \ \ldots$$

2) We are interested in the slow dynamics of x and therefore use homogenization theory to average over the fast dynamics of the velocity v.

3) This results in a partial differential equation for a probability density function $p_0(x)$.

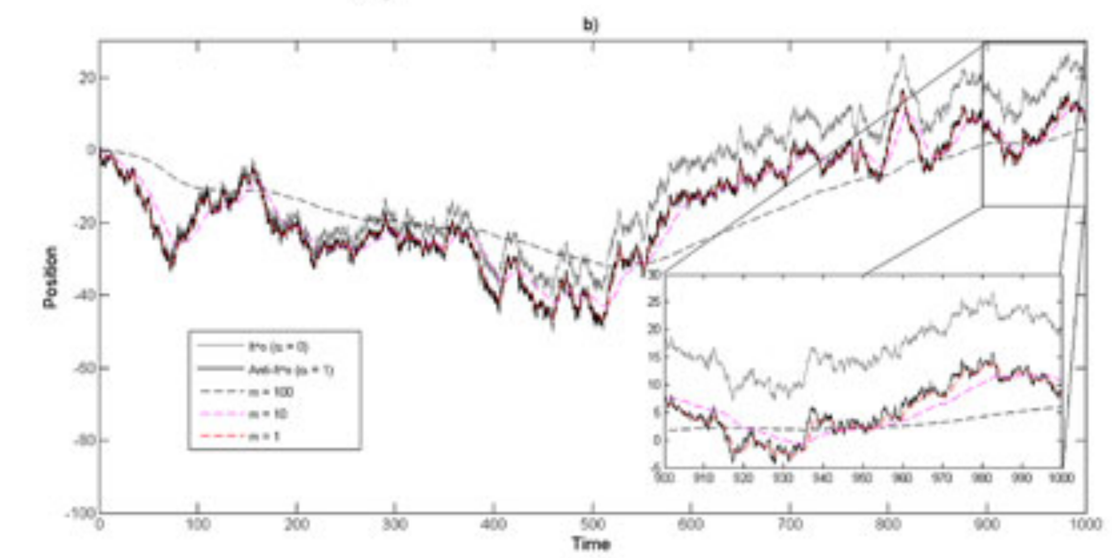
4) This density function leads to a random process $x(t)$ which satisfies a stochastic differential equation.

$$\begin{array}{ccc} \text{SDE } \{x^m(t)\} & \Rightarrow & \text{SDE } \{x(t)\} \\ \downarrow & & \uparrow \\ \text{BK } p_m(x,v) & \longrightarrow & \text{BK } p_0(x) \end{array}$$

Results

The resulting stochastic differential equation includes an extra term accounting for the thermal noise.

$$x(t) = x(0) + \int_0^t \frac{F(x(t))D(x(t))}{k_BT}\,dt + \int_0^t D'(x(t))\,dt + \int_0^t \sqrt{2D(x(t))}\,dW(t)$$



Numerical simulations in MATLAB, show convergence to this process as well.

Conclusion

This work gives a mathematical derivation for the phenomenon seen in the experiments conducted by [1]. Furthermore, for any generic system with friction, $\gamma(x)$, and noise $\sigma(x)$, we give a systematic approach to find the limiting Smoluchoski-Kramers approximation. This results in adding an additional noise induced drift term,

$$\text{Noise induced drift} = \frac{\gamma'(x)\sigma(x)}{2(\gamma'(x)\sigma(x) - \gamma(x)\sigma'(x))}\sigma'(x)\sigma(x)$$

Future work with this small mass limit includes studying the dynamics of the velocity as $m \to 0$ and using a short correlation time for the random noise.

References

[1] G. Volpe, L. Helden, T. Brettschneider, J. Wehr, C. Bechinger, Phys. Rev. Lett. **104**, 170602 (2010)

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