Evolution of the velocity

Starting from SDE

$$\boxed{M \frac{dV}{dt} = - M\gamma V(t) + F_L(t)}$$

we obtain that for each microscopic realization (where $F_L(t)$ assumes a particular form)

$$V(t) = V(t_0)\, e^{-\gamma (t-t_0)} + \frac{1}{M} \int_{t_0}^{t} dt'\, e^{-\gamma(t-t')} F_L(t')$$

homogeneous solution inhomogeneous solution

Such that on average we get

$$\langle v(t) \rangle = \langle v(t_0) \rangle\, e^{-\gamma (t-t_0)}$$

describing an exponential relaxation of the initial velocity towards zero on a time scale $\sim 1/\gamma$, due to Drag force

Similarly, we can obtain the same result by directly looking at evolution equation for the expectation value

$$M \frac{d}{dt} \langle v(t) \rangle = - M \gamma \langle v(t) \rangle$$

$\Downarrow$ yielding the same solution

Based on the general solution of ODE, we can now also look at fluctuations of the velocity around its mean value

$$\delta v(t) = v(t) - \langle v(t) \rangle$$

for which we obtain

$$\delta v(t) = \underbrace{\left(v(t_0) - \langle v(t_0) \rangle \right)}_{\equiv \delta v(t_0)} e^{-\gamma(t-t_0)} + \frac{1}{M} \int_{t_0}^{t} dt' \, e^{-\gamma(t-t')} \bar{f}_L(t')$$

Clearly $\langle \delta v(t) \rangle = 0$ by definition, however the fluctuations are non-zero, as quantified by the equal time auto-correlation function

$$\langle \delta v(t)\, \delta v(t) \rangle = \langle \delta v(t_0)^2 \rangle e^{-2\gamma(t-t_0)}$$

$$+ \frac{1}{M^2} \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' \, e^{-\gamma(t-t')} e^{-\gamma(t-t'')} \langle F_L(t') F_L(t'') \rangle$$

and depend on the auto-correlation function of the stochastic force

Specifically, if we approximate

$$\langle F_L(t') F_L(t'') \rangle = 2 D_v M^2 \delta(t'-t'')$$

we can evaluate for $t > t_0$

$$\frac{1}{m^2}\int_{t_0}^{t} dt' \int_{t_0}^{t} dt''\, e^{-\gamma(t-t')} e^{-\gamma(t-t'')} \langle F_L(t') F_L(t'') \rangle$$

$$= 2D_v \int_{t_0}^{t} dt' \int_{t_0}^{t} dt''\, e^{-\gamma(t-t')} e^{-\gamma(t-t'')}\, \delta(t'-t'')$$

$$= 2D_v \int_{t_0}^{t} dt'\, e^{-2\gamma(t-t')}$$

$$= \frac{D_v}{\gamma}\left(1 - e^{-2\gamma(t-t_0)}\right)$$

So we get

$$\langle \delta v(t)^2 \rangle = \underline{\langle \delta v(t_0)^2 \rangle e^{-2\gamma(t-t_0)}} + \underline{\frac{D_v}{\gamma}\left(1 - e^{-2\gamma(t-t_0)}\right)}$$

Such that the initial fluctuations decay exponentially while new fluctuations are created due to the stochastic force

Specifically at early times $(t-t_0) \ll \frac{1}{\gamma}$ the new fluctuations grow linearly with time

$$\frac{D_v}{\gamma}\left(1-e^{-2\gamma(t-t_0)}\right) \overset{(t-t_0)\ll\frac{1}{\gamma}}{\approx} 2D_v\,(t-t_0)$$

while at late times $(t-t_0) \gg \frac{1}{\gamma}$ the new fluctuations dominate

$$\langle \delta v(t)^2 \rangle \overset{(t-t_0)\gg\frac{1}{\gamma}}{\simeq} \frac{D_v}{\gamma}$$

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Based on $\langle \delta v^2(t) \rangle$, we can also infer the average kinetic energy of the heavy particle as

$$\langle E_{kin}(t) \rangle = \left\langle \frac{1}{2} M v^2(t) \right\rangle \overset{(t-t_0) \gg \frac{1}{\gamma}}{\simeq} \left\langle \frac{1}{2} M \, \delta v^2(t) \right\rangle = \frac{M D_v}{2\gamma}$$

Now in the limit $(t-t_0) \gg \frac{1}{\gamma}$ we expect that the fluid and the heavy particle are in equilibrium with each other, such that the average kinetic energy of the heavy particle is determined by the equipartition theorem

$$\langle E_{kin}(t) \rangle = \frac{k_B T}{2} \quad (\text{in 1D})$$

where T is the temperature of the fluid

So in order to ensure the correct late time limit, the velocity diffusion constant D_v (characterizing the strength of the stochastic force) and the damping rate γ (characterizing the strength of the drag force) need to be related by

$$D_v = \frac{k_B T}{M} \gamma$$

which is called a fluctuation-dissipation relation, which relates properties of dissipative and stochastic terms in the equations of motion

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Besides equal time auto-correlation function $\langle \delta v(t)^2 \rangle$, we can also investigate un-equal time correlation functions, such as e.g. $\langle \delta v(t)\, \delta v(t') \rangle$, which tells us how velocity fluctuations at different times are correlated with each other

Generally we obtain

$$\langle \delta v(t)\, \delta v(t') \rangle = \langle \delta v(t_0)^2 \rangle\, e^{-\gamma(t-t_0)}\, e^{-\gamma(t'-t_0)}$$

$$+ \frac{1}{M^2} \int_{t_0}^{t} d\tilde{t} \int_{t_0}^{t'} d\tilde{\tilde{t}}\, \langle F_L(\tilde{t})\, F_L(\tilde{\tilde{t}}) \rangle\, e^{-\gamma(t-\tilde{t})}\, e^{-\gamma(t'-\tilde{\tilde{t}})}$$

which shows a different sensitivity to auto-correlation of the stochastic force

Specifically for $\langle F_L(\tilde{t}) F_L(\tilde{\tilde{t}}) \rangle = 2D_v M^2 \delta(\tilde{t}-\tilde{\tilde{t}})$

we got for the stochastic contribution

$$2D_v \int_{t_0}^{t} d\tilde{t} \int_{t_0}^{t'} d\tilde{\tilde{t}} \; e^{-\gamma(t-\tilde{t})} e^{-\gamma(t'-\tilde{\tilde{t}})} \; \delta(\tilde{t}-\tilde{\tilde{t}})$$

Now if both $t, t' > t_0$, the constraint $\tilde{t} = \tilde{\tilde{t}}$ of the δ can always be satisfied, as long as $\tilde{\tilde{t}} < t$, so

$$= 2D_v \int_{t_0}^{t'} d\tilde{\tilde{t}} \; e^{-\gamma(t-\tilde{\tilde{t}})} e^{-\gamma(t'-\tilde{\tilde{t}})} \; \theta(t-\tilde{\tilde{t}})$$

and we need to distinguish $t > t'$ and $t < t'$ to perform the $\tilde{\tilde{t}}$ integration

$t > t'$ θ does not give constraint

$$= \frac{D_r}{\gamma} e^{-\gamma t} e^{-\gamma t'} \left[e^{+2\gamma \tilde{t}} \right]_{t_0}^{t'}$$

$$= \frac{D_r}{\gamma} \left[e^{-\gamma(t-t')} - e^{-\gamma(t-t_0)} e^{-\gamma(t'-t_0)} \right]$$

$t < t'$ θ changes range of integration to $\tilde{t} < t$

$$= \frac{D_r}{\gamma} e^{-\gamma t} e^{-\gamma t'} \left[e^{+2\gamma \tilde{t}} \right]_{t_0}^{t}$$

$$= \frac{D_r}{\gamma} \left[e^{+\gamma(t-t')} - e^{-\gamma(t-t_0)} e^{-\gamma(t'-t_0)} \right]$$

Collecting everything we get

$$\langle \delta v(t)\, \delta v(t') \rangle = \langle \delta v^2(t_0) \rangle e^{-\gamma(t-t_0)} e^{-\gamma(t'-t_0)}$$

$$+ \frac{D_v}{\gamma} \left[e^{-\gamma|(t-t')|} - e^{-\gamma(t-t_0)} e^{-\gamma(t'-t_0)} \right]$$

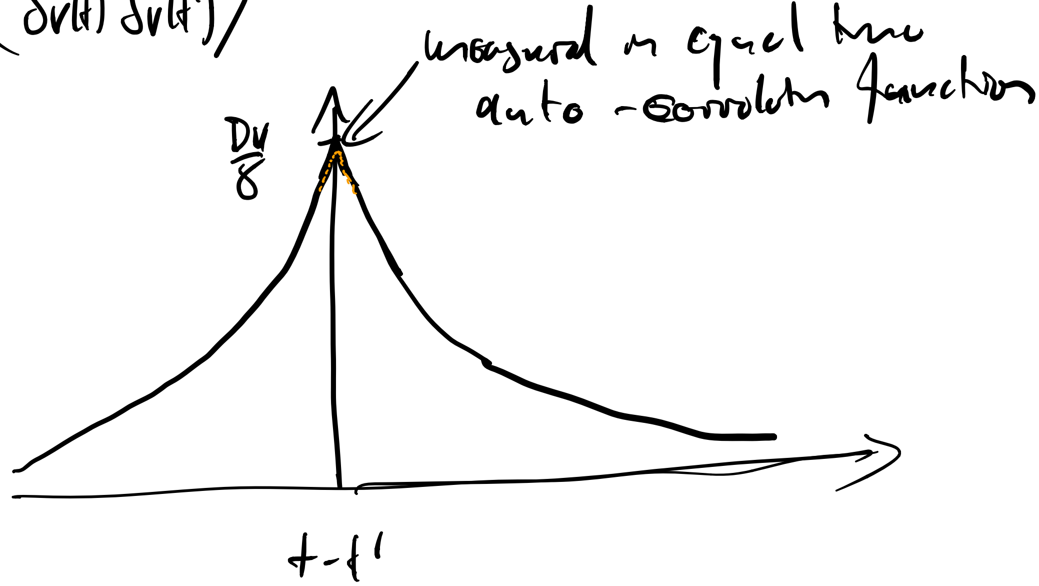
depends on Δt and $\frac{t+t'}{2} - t_0$ which is the average age of the system

Specifically for late times $(t-t_0), (t'-t_0) \gg 1/\gamma$, we have

$$\approx \frac{D_v}{\gamma} e^{-\gamma|(t-t')|}$$

which only depends on the time difference Δt and no longer remembers the initial conditions

$\langle \delta v(t)\, \delta v(t') \rangle$



Non-differentiable behavior at $t=t'$ is a consequence of instantaneous approximation $\mathcal{H}(\Delta t)$ & $\delta(\Delta t)$, which would become smooth for finite collision time

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Evolution of the position

So far we only looked at the evolution of the velocity of the particle, but of course we can also look at the evolution of the average position and its fluctuations

Starting point is again the ODE for the position

$$\frac{d}{dt} X(t) = V(t)$$

together with the solution for the ODE for the velocity $V(t)$ for each microscopic realization

$$V(t) = V(t_0)\, e^{-\gamma (t-t_0)} + \frac{1}{M} \int_{t_0}^{t} dt'\, e^{-\gamma(t-t')}\, F_L(t')$$

So by integration, we obtain that in each microscopic realization

$$X(t) = X(t_0) + \frac{V(t_0)}{\gamma}\left[1 - e^{-\gamma(t-t_0)}\right]$$

$$+ \frac{1}{M}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \, e^{-\gamma(t'-t'')} F_c(t'')$$

changing order of integration

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \overset{t''<t'}{=} \int_{t_0}^{t} dt'' \int_{t''}^{t} dt'$$

we can perform the integration over t'

$$X(t) = X(t_0) + \frac{V(t_0)}{\gamma}\left[1 - e^{-\gamma(t-t_0)}\right]$$

$$+ \frac{1}{M}\int_{t_0}^{t} dt'' \, \frac{1 - e^{-\gamma(t-t'')}}{\gamma} F_c(t'')$$

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If we consider the average displacement the stochastic force does not contribute and we get

$$\langle x(t)\rangle - \langle x(t_0)\rangle = \frac{\langle v(t_0)\rangle}{\gamma}\left[1 - e^{-\gamma(t-t_0)}\right]$$

such that at early times $(t-t_0) \ll 1/\gamma$

<u>ballistic motion:</u> $\langle x(t)\rangle - \langle x(t_0)\rangle = \langle v(t_0)\rangle (t-t_0)$

while at later times $(t-t_0) \gg \frac{1}{\gamma}$

$$\langle x(t)\rangle - \langle x(t_0)\rangle = \frac{\langle v(t_0)\rangle}{\gamma}$$

there is a finite displacement, if the initial velocity is non-zero on average

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Next we can consider fluctuations of the position

$$\delta x(t) = x(t) - \langle x(t) \rangle$$

which are given by

$$\delta x(t) = \underbrace{x(t_0) - \langle x(t_0) \rangle}_{\delta x(t_0)} + \frac{\overbrace{v(t_0) - \langle v(t_0) \rangle}^{\delta v(t_0)}}{\gamma} \left(1 - e^{-\gamma(t-t_0)}\right) + \frac{1}{M} \int_{t_0}^{t} dt' \, \frac{1 - e^{-\gamma(t-t')}}{\gamma} F_c(t')$$

and determine their equal time auto-correlation function to study fluctuations of the position of the heavy particle

$$\langle \delta x(t)\,\delta x(t)\rangle = \langle \delta x(t_0)^2\rangle$$

$$+ 2\left\langle \delta x(t_0)\,\frac{\delta v(t_0)}{\gamma}\right\rangle \left(1-e^{-\gamma(t-t_0)}\right)$$

$$+ \left\langle \frac{\delta v(t_0)^2}{\gamma^2}\right\rangle \left(1-e^{-\gamma(t-t_0)}\right)^2$$

$$+ \langle \delta x(t)\,\delta x(t)\rangle_{F_L}$$

where the contribution from the stochastic force is given by

$$\langle \delta x(t)\,\delta x(t)\rangle_{F_L} =$$

$$\frac{1}{M^2\gamma^2}\int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' \left(1-e^{-\gamma(t-t')}\right)\left(1-e^{-\gamma(t-t'')}\right)\langle F_L(t')\,F_L(t'')\rangle$$

Evaluating this in the instantaneous approximation $\langle F_L(t')\,F_L(t'')\rangle = 2D_v M^2\,\delta(t'-t'')$

$\langle \delta x(t)\,\delta x(t) \rangle_{\xi_L} \simeq$

$$\frac{2 D_v}{\gamma^2}\left[(t-t_0) - \frac{2}{\gamma}\left(1 - e^{-\gamma(t-t_0)}\right) + \frac{1}{2\gamma}\left(1 - e^{-2\gamma(t-t_0)}\right)\right]$$

So if we consider only the contributions from the stochastic force, one finds that for early times $(t-t_0) \ll \frac{1}{\gamma}$

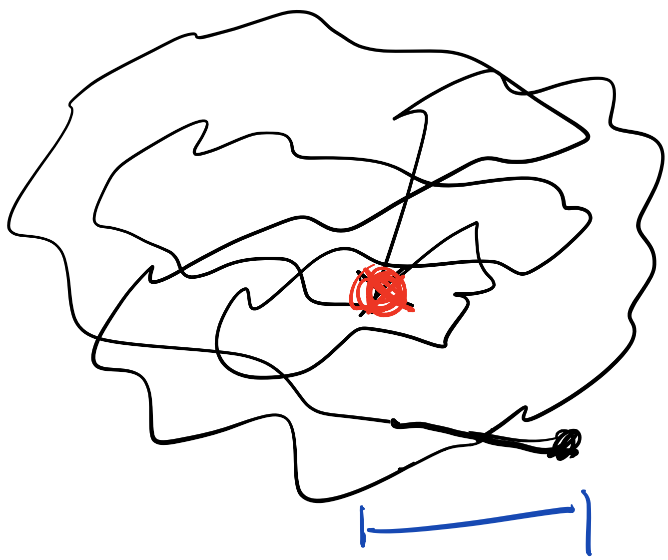
$$\langle \delta x(t)^2 \rangle_{\xi_L} \simeq \frac{2}{3} D_v (t-t_0)^3 \quad \text{for } (t-t_0) \ll \frac{1}{\gamma}$$

where linear and quadratic contributions in $(t-t_0)$ cancel each other between the different terms

Whereas at later times $(t-t_0) \gg \frac{1}{\gamma}$

$$\langle \delta x^2(t) \rangle \simeq \langle \delta x^2(t) \rangle_{\xi_L} = \frac{2 D_v}{\gamma^2}(t-t_0)$$

i.e. the fluctuating force leads to fluctuating velocities, which induce a growing uncertainty in the position of the particle



typical displacement $\delta x \sim \sqrt{\frac{2D_v(t-t_0)}{\gamma^2}}$

By use of the fluctuation dissipation relation $\gamma = \frac{MD_v}{k_BT}$, we can further express the position fluctuations as

$$\langle \delta x(t)^2 \rangle = \frac{2(k_B T)^2}{m^2 D_v}(t-t_0) \quad \text{for } (t-t_0) \gg 1/\gamma$$

Now comparing this with the early time behavior of the velocity auto-correlation function

$$\langle \delta v(t)^2 \rangle - \langle \delta v(t_0)^2 \rangle = 2D_v(t-t_0) \quad \text{for } (t-t_0) \ll 1/\gamma$$

We observe the same linear time dependence of the variance with spatial diffusion constant

$$D_x = \frac{(k_B T)^2}{m^2 D_v}$$

inversely proportional to the velocity diffusion constant

Since the magnitude of velocity fluctuations at late times is fixed by the temperature

$$\langle \delta v(t)^2 \rangle = \frac{k_B T}{M}$$

the diffusion constant D_v only determines the time scale for which the velocity changes, which is encoded in the unequal time auto-correlation function

$$\langle \delta v(t)\, \delta v(t') \rangle \propto e^{-\gamma |t-t'|}$$

Since larger diffusion D_v also implies larger drag γ, the auto-correlation time $1/\gamma$ is shorter, and the particle propagates in a given direction for a shorter period of time resulting in smaller diffusion