V. Stochastic processes

We will discuss basic properties of stochastic processes focusing primarily on Brownian motion of classical particles

Most physical systems are deterministic no randomness involved in describing the dynamics of a system

However to describe dynamics of complex many-body systems, need to keep track of large number of degrees of freedom

Naturally disregarding some degrees of freedom introduces an element of randomness into the description.

→ Stochastic processes are frequently used to model dynamics of complex many-body systems

Physically relevant to a variety of systems, which feature fluctuations due to coarse graining

e.g. thermal fluctuations in fluid
Diffusion processes
Monte Carlo simulations

Central importance also in chemistry, biology & quantitative finance
Black Scholes model

We will focus on the simplest possible example of Brownian motion in one dimension which serves as a good example to illustrate the most important principles

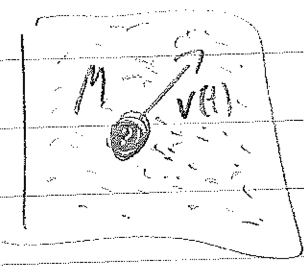
Brownian motion

We consider a heavy particle with mass M moving in a fluid of light particles

e.g. pollen suspended in water

We wish to describe only the dynamics of the heavy particle, eliminating the fluid of light particles from theoretical description

→ introduces element of randomness



$V(t)$ = velocity of heavy particle in rest-frame of fluid

Due to interaction of heavy & light particle there will be forces exerted on the heavy particles

Clearly on average there should be a drag force slowing down the particle which we will model as

$$F_{drag}(t) = -M\gamma V(t)$$

typical example = Stokes friction acting on spherical object in viscous fluid

$$\gamma = 6\pi\eta R$$

Properties of noise term $F_L(t)$

Since the average effect of collisions is already accounted for by drag force

$$\langle F_L(t) \rangle = 0$$

where $\langle \rangle$ denotes an average over different microscopic realizations with same macroscopic properties

However it will lead to fluctuations

$$\langle F_L(t) F_L(t') \rangle = \underbrace{\mathcal{K}(t,t')}_{\text{auto correlation function}}$$

Now if we consider the fluid as stationary, e.g. in global equilibrium the statistical properties of the noise should be time translation invariant

$$\mathcal{K}(t,t') = \mathcal{K}(t-t')$$ only depends on the time difference $|t-t'|$

Note that in higher dimensional systems auto-correlation function becomes a matrix e.g. 3D Brownian motion

$$\langle F_i(t) F_j(t') \rangle = \delta_{ij}\, \mathcal{K}(t-t')$$

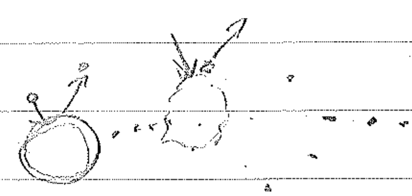
Now what is our picture of the autocorrelation function

Generally when the heavy particle interacts with a light particle, there will be a force exerted over some time τ_{coll} which is the collision time

→ Over $|t-t'| < \tau_{coll}$ the force F_L is due to interactions with a single particle and acts coherently

$$\gamma(t-t') \gg 0$$

Subsequently for $|t-t'| \gg \tau_{coll}$ the particle can encounter interactions with a different light particle

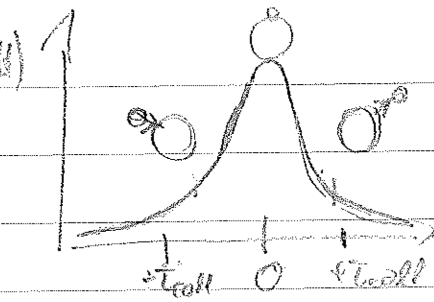


→ Over time scales $|t-t'| \gg \tau_{coll}$ the force comes from interactions with different particles

Since the outcome of individual scattering event is typically independent of each other the force acts incoherently over time scales $|t-t'| \gg \tau_{coll}$

$$\gamma(|t-t'|) \to 0$$

So typically we will have an auto correlation function.



Net effect of these fluctuating forces is quantified by

$$\int_{-\infty}^{\infty} d\Delta t \; \mathcal{K}(\Delta t) = 2 \underbrace{D_v}_{\text{velocity diffusion constant}} M^2$$

Note that if we are interested in the dynamics on time scales $t \gg \tau_{coll}$ it is often sufficient to approximate

$$\mathcal{K}(\Delta t) = 2 D_v M^2 \, \delta(\Delta t)$$

in the spirit of a coarse grained description where the interaction is quasi-instantaneous

Note also that to specify the process completely, we need to specify also the higher order correlation functions $\langle F_L(t_1) \cdots F_L(t_n) \rangle$

One possibility is to assume Gaussian statistics, whereby all n-point functions are determined by auto-correlation function $\mathcal{K}(\Delta t)$ which can be justified by central limit theorem

While this describes the average effect, we expect that microscopically the force on the heavy particle is due to collisions with light particles, where each scattering event will lead to an acceleration of the heavy particle.

Each individual scattering event has an outcome that is in general different from the average, which we can not predict without fuller knowledge on microscopics

Basic idea due to Langevin & Brown is to model the effects of such fluctuations by a stochastic force

$F_L(t)$

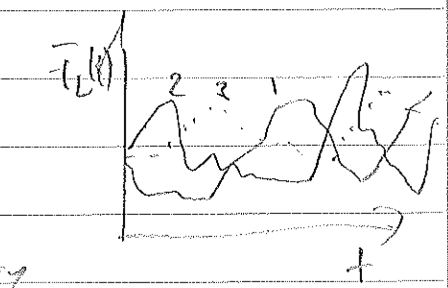
which is randomly distributed according to a certain statistical distribution, but different in each particular realization of the system

Based on these considerations, the dynamics is then described by Newton's law

$$M \frac{dv}{dt} = \sum F = -M\gamma\, v(t) + F_L(t)$$

which involves the stochastic force $F_L(t)$
→ stochastic differential equation

While in every single microscopic realization of the system $F_L(t)$ takes on a particular form and the dynamics is described by an ordinary differential equation for this particular noise term, the macroscopic properties are described by stochastic differential equation which is defined by averaging over all possible microscopic realizations



While generally this is a difficult task, in this particular case it is possible since the SDE is linear and the noise term $F_L(t)$ is independent of the stochastic variable $v(t)$

In order to construct solutions to SDE one has two possibilities

1) Solve ODE for general noise term and subsequently average over all possible realizations

2) Directly construct EOMs for expectation values of interest and solve them

Evolution of velocity:

We have for each microscopic realization for $t > t_0$

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

so on average we get

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

exponential relaxation on a characteristic time scale $\tau = \frac{1}{\gamma}$

Similarly we could have obtained the same result by directly looking at EOM for average

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

We can next look at the velocity fluctuations

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

and first consider the equal time auto-correlation function

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

~~Based on the approximation of auto correlation function~~

$$\mathcal{K}(\Delta t) = 2 D_v M^2\, \delta(\Delta t)$$

we get

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

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

So for instance if actually the velocity is fixed for all various copie realizations e.g. particle always at rest

then $\langle \delta v^2(t)\rangle \simeq 2D_v\,(t-t_0)$ for $(t-t_0) \ll \frac{1}{\gamma}$

for later times initial condition ~~becomes irrelevant~~ and approaches

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

We can also relate the average kinetic energy of the particle

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

Now in the limit $t-t_0 \gg \frac{1}{\gamma}$ we expect that heavy particle and fluid are in equilibrium with each other

$$\langle E_{kin}(t)\rangle = \frac{k_B T}{2}$$

Hence we obtain a relation between D_v and γ

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

Since it relations properties of fluctuating force and dissipative drag force this is an example of

<u>fluctuation dissipation relation</u>

Besides equal time auto-correlation $\langle \delta v(t)^2 \rangle$
we can also calculate other
properties of the process e.g.

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

which tells us how fluctuations of velocity are
correlated over a time scale $\Delta t = |t-t'|$

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

Based on the the approximation ...

$$\gamma(\Delta t) = 2 D_v M^2 \delta(\Delta t)$$

we get that contribution from Langevin force $\Rightarrow$

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

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

note that we dropped the θ-fn from lower bound
since both t, t' are assumed to be larger than t_0

Need to distinguish cases
$t > t'$ and $t < t'$

So for $t > t'$ θ does not provide additional constraint

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

conversely for $t < t'$ the upper bound of integral is set by t

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

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

So we get

$$\langle \delta v(t)\,\delta v(t')\rangle = \langle \delta v^2(t_0)\rangle\, e^{-\gamma(t-t_0)}\, e^{-\gamma(t'-t_0)}$$
$$+ \frac{D_v}{\gamma}\left[e^{-\gamma|t-t'|} - e^{-\gamma(t-t_0)}e^{-\gamma(t'-t_0)}\right]$$

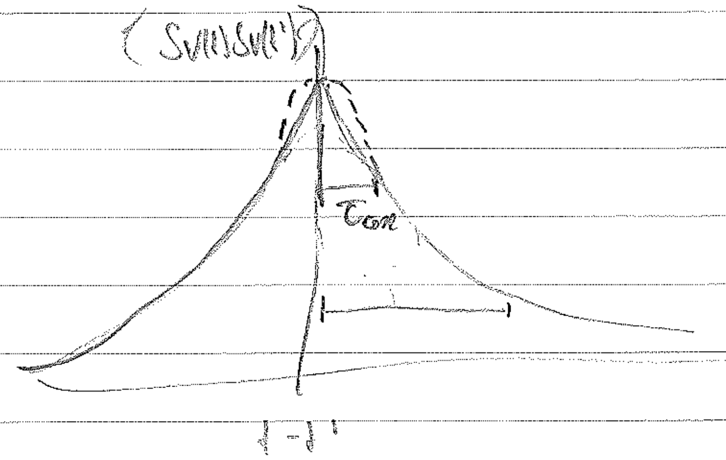
So in particular for $t, t' \gg t_0$
or likewise $\lim_{t_0 \to -\infty}$

$$= \frac{D_v}{\gamma}\, e^{-\gamma|t-t'|}$$

which only depends on the time difference $|\Delta t|$

Similarly the more general expression also depends on $|\Delta t|$ and $\frac{t+t'}{2} - t_0$ which is the

So we get in the limit $t, t' \gg \tau$



Non-differentiable behaviour near $t - t' \approx 0$ can be traced back to instantaneous approximation of autocorrelation function

→ in reality smoothed out over time scale τ_{coll} where velocity changes continuously

So far we only looked at evolution of velocity and its fluctuations

Can now also look at position of particle

Starting point of analysis is given general solution of the ODE for velocity

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

for each microscopic realization

$$x(t) = \int_{t_0}^{t} dt'\, v(t') + x(t_0)$$

so

$$x(t) = x(t_0) + \frac{v_0}{\gamma}\left(1 - e^{-\gamma(t-t_0)}\right) + \frac{1}{M}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, e^{-\gamma(t'-t'')}\, F_L(t'')$$

in the last term such that $t_0 < t'' < t' < t$

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

$$= \frac{1}{M}\int_{t_0}^{\infty} dt'' \left(\int_{t_0}^{t} dt'\, \theta(t'-t'')\, e^{-\gamma(t'-t'')}\right) F_L(t'')$$

$$= \frac{1}{M}\int_{t_0}^{\infty} dt'' \left(\int_{t''}^{t} dt'\, \theta(t-t'')\, e^{-\gamma(t'-t'')}\right) F_L(t'')$$

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

So we got

$$X(t) = X(t_0) + \frac{v_0}{\gamma}\left(1-e^{-\gamma(t-t_0)}\right) + \frac{1}{M}\int_{t_0}^{t} dt'' \, \frac{1-e^{-\gamma(t-t')}}{\gamma} F_L(t')$$

Such that on average

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

which means that for

$$t-t_0 \ll \frac{1}{\gamma} \qquad \langle x(t)\rangle = \langle x(t_0)\rangle + \langle v(t_0)\rangle (t-t_0)$$

ballistic motion

$$t-t_0 \gg \frac{1}{\gamma} \qquad \langle x(t)\rangle = \langle x(t_0)\rangle + \frac{\langle v(t_0)\rangle}{\gamma}$$

finite displacement from original position which is approached exponentially

Next we can consider also the fluctuations

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

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

So we get

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

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

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

$$\langle F_L(t')\, F_L(t'')\rangle$$

So within approximation of auto-correlation function the last term becomes

$$\frac{2D_v}{\gamma^2}\int_{t_0}^{t} dt' \left(1-e^{-\gamma(t-t')}\right)^2$$

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

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

So in particular if there are initially no fluctuations $\delta x(t_0) = 0$ $\delta v(t_0) = 0$ respectively, i.e. position and velocity of particle are known with certainty

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

So for $t - t_0 \ll \frac{1}{\gamma}$ linear and quadratic terms cancel

$$\langle \delta x^2(t) \rangle \simeq \frac{2D_v}{3} t^3$$

in the long time limit $t - t_0 \gg \frac{1}{\gamma}$

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

linear growth as in ordinary diffusion process

We conclude that the coordinate space diffusion constant is given by

$$D = \frac{D_v}{\gamma^2}$$

using fluctuation dissipation relation $\gamma = \frac{M D_v}{k_B T}$

we conclude that $D = \frac{(k_B T)^2}{M^2 D_v}$ is inversely

Spectral analysis

Consider the process in the frequency domain rather than in time domain

Will focus on stationary stochastic processes ie processes where statistical properties of noise are time translation invariant

e.g. $\langle F_L(t) F_L(t') \rangle = \Gamma \delta(t-t')$

Define

$$\tilde{F}_L(\omega) = \int_{-\infty}^{\infty} dt \; F_L(t)\, e^{+i\omega t}$$

$$\tilde{V}(\omega) = \int_{-\infty}^{\infty} dt \; V(t)\, e^{+i\omega t} \qquad V(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \tilde{V}(\omega) e^{-i\omega t}$$

How the EOM reads in ω-space

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

$$-i\omega \tilde{V}(\omega) = -M\gamma \tilde{V}(\omega) + \tilde{F}_L(\omega)$$

So we have

$$\tilde{V}(\omega) = \frac{1}{M} \frac{1}{\gamma - i\omega} \tilde{F}_L(\omega)$$

We can thus look at the auto-correlation function

$$\langle F_L(t) F_L(t') \rangle = \mathcal{K}(t-t')$$

$$\langle \tilde{F}_L(\omega) \tilde{F}_L^*(\omega') \rangle = \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' \, \langle F_L(t) F(t') \rangle \, e^{i\omega t} e^{-i\omega' t'}$$

So for stationary process

$$\Delta t = t - t' \qquad T = \frac{t+t'}{2}$$

$$= \int_{-\infty}^{\infty} d\Delta t \int_{-\infty}^{\infty} dT \; \mathcal{K}(\Delta t) \, e^{i\omega\left(T + \frac{\Delta t}{2}\right)} e^{-i\omega'\left(T - \frac{\Delta t}{2}\right)}$$

$$= \int_{-\infty}^{\infty} d\Delta t \; \mathcal{K}(\Delta t) \, e^{i\omega \Delta t} (2\pi) \delta(\omega - \omega')$$

$$= 2\pi \, \delta(\omega - \omega') \, \tilde{\mathcal{K}}(\omega)$$

Specifically for instantaneous approximation of noise we have

$$\mathcal{K}(\Delta t) = 2 D_v M^2 \delta(\Delta t)$$

$$\Rightarrow \tilde{\mathcal{K}}(\omega) = 2 D_v M^2 \qquad \text{(independent of } \omega\text{)}$$

noise is spectrally white, i.e. all frequency components are equally weighted

So we get for the auto-correlation function of the velocity (for stationary stochastic process)

$$\langle \tilde{V}(\omega)\, \tilde{V}^*(\omega') \rangle = \frac{1}{M^2} \frac{1}{\gamma^2+\omega^2} \tilde{\xi}(\omega)\, (2\pi)\, \delta(\omega-\omega')$$

Specifically for white noise

$$= \frac{2D_V}{\gamma^2+\omega^2} (2\pi)\, \delta(\omega-\omega')$$

$\Rightarrow$ while all frequencies are served equally by the noise term the system responds differently to different frequency excitations

Can use this result to reconstruct auto-correlation function in time domain

Inverse FT

$$V(t) = \int_{-\infty}^{\infty} \frac{d\omega}{(2\pi)} \tilde{f}_L(\omega)\, e^{-i\omega t} = \int_{-\infty}^{\infty} \frac{d\omega}{(2\pi)} \tilde{f}_L^*(\omega)\, e^{i\omega t}$$

complex conjugation

$$\langle V(t)\, V(t+\Delta t) \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{(2\pi)} \int_{-\infty}^{\infty} \frac{d\omega'}{(2\pi)} \langle V(\omega)\, V^*(\omega') \rangle\, e^{-i\omega t}\, e^{+i\omega'(t+\Delta t)}$$

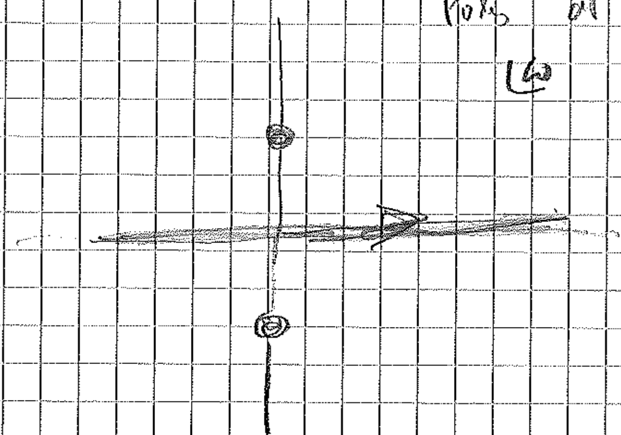
stationary process

$$= \int_{-\infty}^{\infty} \frac{d\omega}{(2\pi)} \frac{\tilde{\xi}(\omega)}{M^2} \frac{1}{\gamma^2+\omega^2} e^{i\omega\Delta t}$$

So lets verify that we get the same for white noise

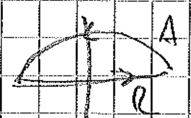
$$\langle V(t)\, V(t+\Delta t)\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{(2\pi)} \frac{2D_v}{\gamma^2+\omega^2}\, e^{i\omega\Delta t}$$

Poles at $\omega = \pm i\gamma$



Can use contour integral technique

So for $\Delta t > 0$ can close contour



such that on A $\mathrm{Im}(\omega) > 0$

$\mathrm{Re}(i\omega\Delta t) < 0$

Contour A does not give contribution

$\Rightarrow$ integral is then given by the residue at the pole of integrand

$$\frac{1}{\gamma^2+\omega^2} = \frac{1}{(\omega-i\gamma)}\,\frac{1}{(\omega+i\gamma)}$$

So for $\Delta t > 0$ we pick up pole at $\omega = i\gamma$

We get for $\Delta t > 0$

$\underline{\Delta t > 0}$ $$\langle v(t)\, v(t+\Delta t)\rangle = \underset{\text{residue theorem}}{(2\pi i)} \left.\frac{2D_v}{\omega + i\gamma}\, e^{i\omega\Delta t}\right|_{\omega = i\gamma}$$

$$= \frac{D_v}{\gamma}\, e^{-\gamma\Delta t}$$

Here we need for $\Delta t < 0$ need to close contour in the other direction.

$\underline{\Delta t < 0}$: $$\langle v(t)\, v(t+\Delta t)\rangle = -\underset{\substack{\text{residue theorem} \\ \text{with contour} \\ \text{large on} \\ \text{opposite way}}}{(2\pi i)} \left.\frac{2D_v}{\omega - i\gamma}\, e^{i\omega\Delta t}\right|_{\omega = -i\gamma}$$

$$= \frac{D_v}{\gamma}\, e^{+\gamma\Delta t}$$

So in Summary

$$\langle v(t)\, v(t+\Delta t)\rangle = \frac{D_v}{\gamma}\, e^{-\gamma|\Delta t|}$$

Which gives the long time limit of our previous result

Note that in order to perform full Fourier transform we had to send $t_0 \to -\infty$,

In this limit the initial condition is in the infinite past and the system is in equilibrium at any finite time