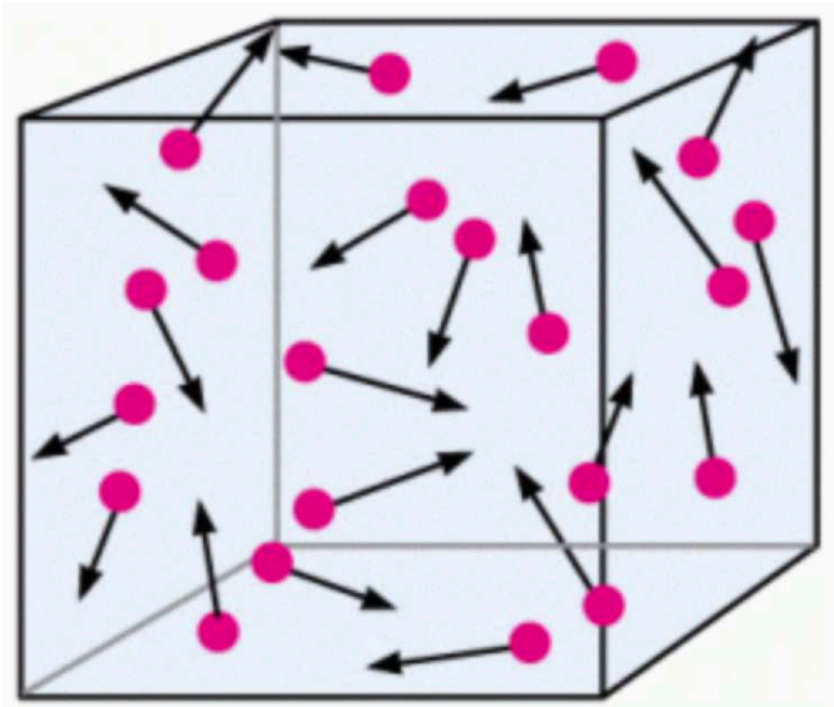
LECTURE 7

Stochasticity & the Langevin Equation

Part II: Kinetic Theory



Part II: Kinetic Theory

Preliminaries

Random Variable: a (1-dimensional) random variable is a scalar function $x(t)$, where t is usually time, for which the future evolution is not determined by any set of initial data knowable to us.

Random Process: (aka stochastic process) is an ensemble of realizations of random variables $x(t)$, that all represent the same physical entity. Any particular $x(t)$ is called a realization of the random process.

In general, a random process is completely specified by the following *set* of probability functions:

$$
\begin{aligned}
P_1 &= P_1(x_1, t_1)\mathrm{d}x_1 \\
P_2 &= P_2(x_2, t_2; x_1, t_1)\mathrm{d}x_2\,\mathrm{d}x_1 \\
&. \\
&. \\
P_n &= P_n(x_n, t_n, ..., x_2, t_2, x_1, t_1)\mathrm{d}x_n \ldots \mathrm{d}x_2\,\mathrm{d}x_1
\end{aligned}
$$

Ensemble Averages: the ensemble average of a function $f(x(t))$ of a random variable is defined as

$$\langle f(t) \rangle = \int f(x)\, P_1(x,t)\, \mathrm{d}x$$

Preliminaries

Similarly, we can also compute the ensemble averages that involve multiple epochs, such as

$$\langle x(t_1)x(t_2)\rangle = \int x_1\, x_2\, P_2(x_2, t_2; x_1, t_1)\, \mathrm{d}x_2 \mathrm{d}x_1$$

Stationarity: a random process is said to be **stationary** iff its probability distributions P_n (for all n) depend only on time differences and not on absolute time, i.e.,

$$P_n(x_n, t_n + \tau; ...; x_2, t_2 + \tau; x_1, t_1 + \tau) = P_n(x_n, t_n, ..., x_2, t_2, x_1, t_1) \qquad \forall \tau$$

Ergodicity: Let $f(x)$ be any function of a random variable $x(t)$. A stationary random process is said to be ergodic iff the time average of a realization,

$$\overline{f} = \lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} f[x(t')]\, \mathrm{d}t'$$

is equal to the ensemble average $\langle f(x)\rangle$.

Preliminaries

For $f(x) = x$, ergodicity means that the time average of a given realization (when averaged over a sufficiently long time) is equal to the ensemble average over many realizations

Markov Process: a random process is said to be Markov (or 'Markovian') iff all future probabilities are determined completely by its most recently known values, i.e.,

$$P_n(x_n, t_n | x_{n-1}, t_{n-1}; ...; x_2, t_2; x_1, t_1) = P_2(x_n, t_n | x_{n-1}, t_{n-1})$$

Bayes Theorem: $P(A,B) = P(A|B)\,P(B) = P(B|A)\,P(A)$ → $P(A|B) = \frac{P(A,B)}{P(B)} = \frac{P(B|A)\,P(A)}{P(B)}$

Hence we have that

$$P_n(x_n, t_n | x_{n-1}, t_{n-1}; ...; x_2, t_2; x_1, t_1) = \frac{P_n(x_n, t_n; x_{n-1}, t_{n-1}; ...; x_2, t_2; x_1, t_1)}{P_{n-1}(x_{n-1}, t_{n-1}; ...; x_2, t_2; x_1, t_1)}$$

which impies that a stationary Markov process is completely specified by

$$P_1(x) \quad \text{and} \quad P_2(x_2, t | x_1) = \frac{P_2(x_2, t; x_1, 0)}{P_1(x_1)}$$

The Langevin Equation

Consider a collisional N-body system, and lauch particles with phase-space coordinates $(\boldsymbol{q}_0,\boldsymbol{p}_0)$ at different times t_i

Each of these particles will execute different trajectories, $\mu_i(t) = (\boldsymbol{q}(t),\boldsymbol{p}(t))$ in phase-space due to the fact that the forces, $\boldsymbol{F}(t)$, it experiences are stochastic

In other words, $\boldsymbol{F}(t)$, is a random variable, and as a consequence, so is $\mu(t)$

The stochasticity is a manifestation of collisions with all the other particles.

Hamiltonian systems are deterministic, and this stochasticity is only a consequence of not knowing the exact microstate corresponding to the macrostate of the system

Let $<\mu(t)>$ be the ensemble average trajectory

We can write:

$$\vec{F}(\vec{x},t) = \langle \vec{F}(\vec{x}) \rangle + \delta \vec{F}(\vec{x},t)$$

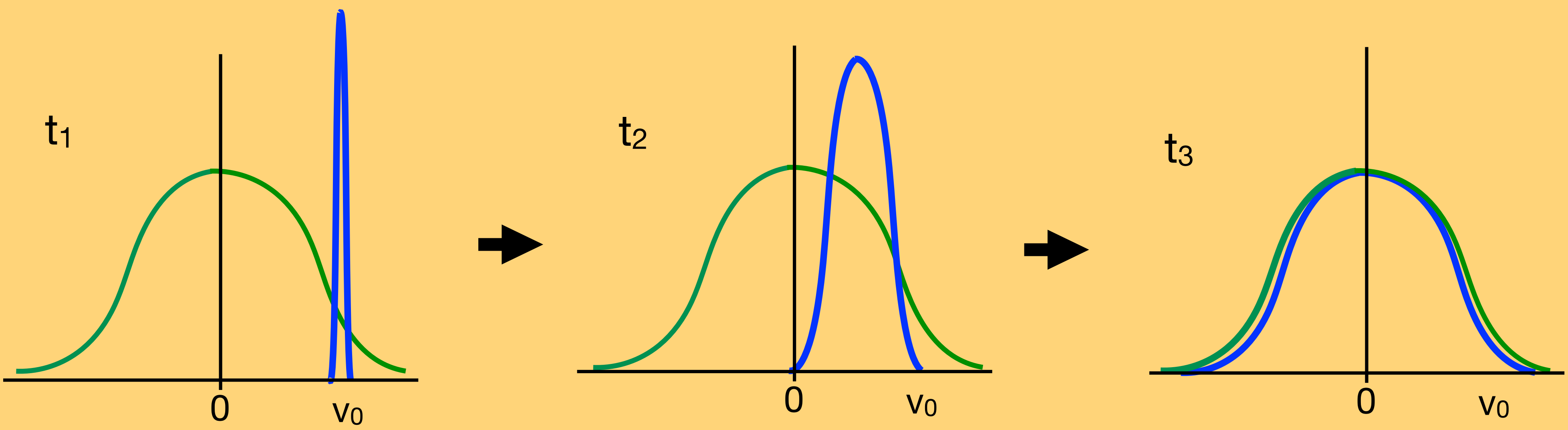
where $<\boldsymbol{F}(x)>$ is the force field that gives rise to $<\mu(t)>$, and the residual $<\delta\boldsymbol{F}(x,t)>$ is the stochastic force, for which $<\delta\boldsymbol{F}>=0$

The Langevin Equation

We can write $\langle \boldsymbol{F}(x) \rangle$ as the sum of a velocity-independent, conservative force, $\boldsymbol{F}_c(\boldsymbol{x}) = -\nabla V(\boldsymbol{x})$, and a velocity-dependent force, $\boldsymbol{F}_{nc}(\boldsymbol{x}, t)$

The velocity-dependent component manifests as a friction force.

Hence, $\langle \mu(t) \rangle$ is NOT the same as the trajectory in the absence of stochastic forces !!!



Evolution of an ensemble of particles in a thermal bath

Note that particles experience both friction ($\langle v \rangle$: $v_0 \rightarrow 0$) as well as diffusion

The Langevin Equation

In what follows, we ignore spatial dependence; we assume a homogeneous sea of particles of density ρ, and we will assume that the impact of stochasticity at $\boldsymbol{x}$ where the density is $\rho(\boldsymbol{x})$ is identical to the impact it would experience in a homogeneous sea of that density.

This is known as the **local approximation**, which is common in gravitational N-body systems

Using Taylor series expansion, and making the local approximation, we have that

$$F_{\rm nc}(\vec{x},\vec{v}) = F_{\rm nc}(v) = c_0 + c_1\,v + c_2\,v^2 + \mathcal{O}(v^3)$$

Since velocity-independent force is already accounted for by $\boldsymbol{F}_c(\boldsymbol{x}) = -\nabla V(\boldsymbol{x})$, we have that $c_0=0$

Let's truncate series at first order, so that equation of motion for our subject mass becomes

$$m\,\frac{{\rm d}\vec{v}}{{\rm d}t} = \vec{F}(\vec{x},t) = -\nabla V(\vec{x}) - \gamma\vec{v}(t) + \delta\vec{F}(t)$$

where we have replaced c_1 by γ, which is called the friction coefficient   ($[\gamma]$ = g s^{-1})

The quantity $1/\gamma$ is sometimes called the mobility

The equation of motion is a stochastic differential equation, known as the Langevin equation

It differs from ordinary differential equations in that it contains a stochastic term, $\delta\boldsymbol{F}(t)$.

It has a different solution for each realization of the random process.

The Langevin Equation

What are you supposed to do with a stochastic equation, like the Langevin equation?

You try to solve for the ensemble average, <μ(*t*)>, using statistical properties of the random process; in this case, statistical properties of $\delta \boldsymbol{F}(t)$

Because of our assumption of homogeneity, we actually have that $\nabla V(\boldsymbol{x}) = 0$.

If we further simplify matters by considering a 1D system, the Langevin eq. simplifies to

$$m\,\frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = \vec{F}(\vec{x},t) = -\nabla V(\vec{x}) - \gamma\vec{v}(t) + \delta\vec{F}(t) \quad \Rightarrow \quad m\frac{\mathrm{d}v}{\mathrm{d}t} = -\gamma v + \delta F(t)$$

Multiplying by $\exp(\gamma t/m)$ and rearranging yields

$$\frac{\mathrm{d}v}{\mathrm{d}t}\mathrm{e}^{\gamma t/m} + \frac{\gamma}{m}v\mathrm{e}^{\gamma t/m} = \frac{\mathrm{d}}{\mathrm{d}t}\left[v\mathrm{e}^{\gamma t/m}\right] = \frac{1}{m}\delta F(t)\,\mathrm{e}^{\gamma t/m}$$

which is easily solved: $$v(t) = v_0\,\mathrm{e}^{-\gamma t/m} + \frac{1}{m}\int_0^t \delta F(t')\,\mathrm{e}^{-\gamma(t'-t)/m}\,\mathrm{d}t'$$

The Langevin Equation

$$v(t) = v_0\,\mathrm{e}^{-\gamma t/m} + \frac{1}{m}\int_0^t \delta F(t')\,\mathrm{e}^{-\gamma(t'-t)/m}\,\mathrm{d}t'$$

Taking the ensemble average, and using that $<\delta \boldsymbol{F}>=0$, we obtain

$$\langle v(t)\rangle = v_0\,\mathrm{e}^{-\gamma t/m}$$

Hence, the ensemble average decays to zero on a `dissipation' time $\tau_{\mathrm{d}} = m/\gamma$

NOTE: it is called a dissipation time, because a decrease in kinetic energy implies a decrease in energy (recall that V=0). This may sound confusing, given that we are working with Hamiltonian systems, which are non-dissipative. However, the energy is transferred to other particles, though, so there is no net dissipation.

Let's now solve for the ensemble average of the trajectory:

$$\langle x(t)\rangle = x_0 + \int_0^t \mathrm{d}t'\,\langle v(t')\rangle = x_0 + \frac{m}{\gamma} v_0\,(1 - \mathrm{e}^{-\gamma t/m})$$

As expected, this represents a particle that moves in a straight line with a velocity that is decaying with time…

The Langevin Equation

But we can also compute more complicated ensemble averages, for example the correlation between the velocities at different times:

$$\langle v(t_1)v(t_2)\rangle = \langle v(t_1)\rangle \langle v(t_2)\rangle + \frac{1}{m^2}\int_0^{t_1} \mathrm{d}t_1' \int_0^{t_2} \mathrm{d}t_2' \, \langle \delta F(t_1')\, \delta F(t_2')\rangle \, \mathrm{e}^{\gamma(t_1'+t_2'-t_1-t_2)/m}$$

Here again we have used the fact that $<\delta \boldsymbol{F}>=0$ to drop the cross terms

As is evident, in order to compute the correlation between the velocities, we need to know how the stochastic forces are correlated.

Typically, if $t_2 - t_1 \gg \tau_{\rm coll}$ then the forces will be uncorrelated, i.e., $<\delta \boldsymbol{F}(t_1)\ \delta \boldsymbol{F}(t_2)>=0$

If $\tau_{\rm coll}$ is much shorter than any other timescale of interest, we can effectively take the limit $\tau_{\rm coll} \rightarrow 0$, for which $\langle \delta F(t_1)\, \delta F(t_2)\rangle = 2D\,\gamma^2\,\delta(t_2 - t_1)$

Here the factor γ^2 has been put in for convenience, and D characterizes the strength of the correlation. It is called the diffusion coefficient ($[D] = \mathrm{cm}^2\ \mathrm{s}^{-1}$) as will become evident.

A stochastic variable x that obeys $<x(t_1)\ x(t_2)> \propto \delta(t_2 - t_1)$ is referred to as white noise

The Langevin Equation

$$\langle v(t_1)v(t_2)\rangle = \langle v(t_1)\rangle\,\langle v(t_2)\rangle + \frac{1}{m^2}\int_0^{t_1} \mathrm{d}t_1' \int_0^{t_2} \mathrm{d}t_2'\, \langle \delta F(t_1')\,\delta F(t_2')\rangle\, \mathrm{e}^{\gamma(t_1'+t_2'-t_1-t_2)/m}$$

Substituting $\langle \delta F(t_1)\,\delta F(t_2)\rangle = 2D\,\gamma^2\,\delta(t_2-t_1)$ yields

$$\begin{aligned}\langle v(t_1)v(t_2)\rangle &= \langle v(t_1)\rangle\,\langle v(t_2)\rangle + \frac{2D\gamma^2}{m^2}\,\mathrm{e}^{-\gamma(t_1+t_2)/m}\int_0^{t_1}\mathrm{d}t'\mathrm{e}^{2\gamma t'/m} \\ &= \langle v(t_1)\rangle\,\langle v(t_2)\rangle + \frac{D\gamma}{m}\left[\mathrm{e}^{-\gamma(t_1-t_2)/m} - \mathrm{e}^{-\gamma(t_1+t_2)/m}\right]\end{aligned}$$

In the limit $t\rightarrow\infty$ we can drop the last term, as well as $\langle v(t_1)\rangle\,\langle v(t_2)\rangle$ since $v\rightarrow 0$, hence

$$\langle v(t_1)v(t_2)\rangle \underset{t_1,t_2\rightarrow\infty}{\longrightarrow} \frac{D\gamma}{m}\,\mathrm{e}^{-\gamma(t_2-t_1)/m}$$

Using that we assume stochastic force to be stationary, we can rewrite this as

$$\langle v(t)v(t+\Delta t)\rangle \underset{t\rightarrow\infty}{\longrightarrow} \frac{D\gamma}{m}\,\mathrm{e}^{-\gamma\Delta t/m}$$

Hence, velocities are correlated but only for a short period; they become uncorrelated again on the dissipation time $\tau_d = m/\gamma$. This justifies Boltzmann's molecular chaos ansatz

The Einstein-Smoluchowski Equation

Reverting back from 1D to 3D, this becomes $\langle \vec{v}(t) \cdot \vec{v}(t) \rangle = \langle v^2(t) \rangle \underset{t \to \infty}{\longrightarrow} \frac{3D\gamma}{m}$

Hence, after a sufficiently long time the velocity dispersion among particles that all started from an identical point in phase-space, is given by

$$\sigma_v^2 = \langle v^2 \rangle - \langle v \rangle^2 = \frac{3D\gamma}{m}$$

Thus we see that the velocity dispersion asymptotes to a constant value!!!

We know that collisions drive the system towards equipartition, in which the kinetic energy of the subject mass becomes equal to that of the field particles:

$$\frac{1}{2} m \langle v^2 \rangle = \tfrac{3}{2} k_{\rm B} T$$

We thus infer that

$$\boxed{D\gamma = k_{\rm B} T}$$

valid as long as field particles are thermal bath in thermal equilibrium

which is known as the Einstein-Smoluchowski relation. It shows that the diffusion coefficient and the friction coefficient are closely related

This is a manifestation of the fluctuation-dissipation theorem, which basically states that fluctuating forces cause dissipation (friction)

The Smoluchowski Equation

Consider three arbitrary times: $t_3 > t_2 > t_1$ and let $x(t)$ be a random process

We can alway write that

$$P_2(x_3, t_3|x_1, t_1) = \int P_3(x_3, t_3|x_2, t_2; x_1, t_1)\, P_2(x_2, t_2|x_1, t_1)\, \mathrm{d}x_2$$

which simply states that as x transitions from x_1 at t_1 to x_3 at t_3, it must pass through some x_2 at t_2

Iff the random process is Markovian and stationary, we have that

$$P_3(x_3, t_3|x_2, t_2; x_1, t_1) = P_2(x_3, t_3|x_2, t_2) = P_2(x_3, t_3 - t_2|x_2)$$

In this case the expression simplifies to

$$\boxed{P_2(x_3, t_3|x_1) = \int P_2(x_3, t_3 - t_2|x_2)\, P_2(x_2, t_2|x_1)\, \mathrm{d}x_2}$$

known as the Smoluchowski equation (or the Chapman-Kolmogorov equation)

From Smoluchowski Equation to Fokker-Planck

$$P_2(x_3, t_3|x_1) = \int P_2(x_3, t_3 - t_2|x_2)\, P_2(x_2, t_2|x_1)\, \mathrm{d}x_2$$

$$t_3 \to t + \Delta t$$
$$x_3 \to x$$
$$x_2 \to x - \Delta x$$
$$x_1 \to x_0$$

$$\boxed{P_2(x, t + \Delta t) = \int \Psi(\Delta x, \Delta t | x - \Delta x, t)\, P_2(x - \Delta x, t|x_0)\mathrm{d}(\Delta x)}$$

only valid for stationary, Markovian random process

where $\Psi(\Delta x, \Delta t|x - \Delta x, t) = P_2(x, t + \Delta t|x - \Delta x, t)$ is the transition probability that starting from $x - \Delta x$ at t the random variable undergoes a change Δx in timestep Δt

Using a Taylor series expansion for the integrant in the above expression, we obtain

$$\begin{aligned}
P_2(x, t + \Delta t) &= \int \mathrm{d}(\Delta x) \sum_{n=0}^{\infty} \frac{(-\Delta x)^n}{n!} \frac{\partial^n}{\partial x^n} \left[\Psi(\Delta x, \Delta t|x - \Delta x, t)\, P_2(x - \Delta x, t|x_0)\right]_{x - \Delta x = x} \\
&= \int \mathrm{d}(\Delta x) \sum_{n=0}^{\infty} \frac{(-\Delta x)^n}{n!} \frac{\partial^n}{\partial x^n} \left[\Psi(\Delta x, \Delta t|x, t)\, P_2(x, t|x_0)\right] \\
&= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial x^n} \left[P_2(x, t|x_0) \int \mathrm{d}(\Delta x)\, (\Delta x)^n\, \Psi(\Delta x, \Delta t|x - \Delta x, t)\right] \\
&= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial x^n} \left[\langle(\Delta x)^n\rangle\, P_2(x, t|x_0)\right]
\end{aligned}$$

From Smoluchowski Equation to Fokker-Planck

Using that the n=0 term in the Taylor series expansion is nothing but $P_2(x,t|x_0)$ we obtain

$$\begin{aligned}\frac{\partial P_2(x,t|x_0)}{\partial t} &= \lim_{\Delta t\to 0}\frac{P_2(x,t+\Delta t|x_0)-P_2(x,t|x_0)}{\Delta t}\\ &= \sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{\partial^n}{\partial x^n}\left[D^{(n)}(x,t)\,P_2(x,t|x_0)\right]\end{aligned}$$

where we have defined $\boxed{D^{(n)}(x,t) \equiv \lim_{\Delta t\to 0}\frac{\langle(\Delta x)^n\rangle}{\Delta t}}$

If we only keep the first two terms in the Taylor series expansion (i.e., we assume that Δx is small enough such that the higher order terms can be ignored), then we obtain the

Fokker-Planck equation $\boxed{\frac{\partial P_2}{\partial t} = -\frac{\partial}{\partial x}[D^{(1)}P_2] + \frac{1}{2}\frac{\partial^2}{\partial x^2}[D^{(2)}P_2]}$

This is a generalized diffusion equation for the evolution of P_2