Module 2 – Statistical Dynamics I

This Module: Basics of Statistical Dynamics (more later)

- Thermal Equilibrium Fluctuations
- Brownian Motion

- Fluctuation–Dissipation Theorem 1

⇒

- Fokker–Planck Theory

Several topics will be investigated in depth when we are further along in the course

L 1a { Thermal Equilibrium Fluctions, F-D Theorem, Brownian Motion

→ Simplest possible stochastic dynamics problem:

Brownian Motion:

Robert Brown, 1827

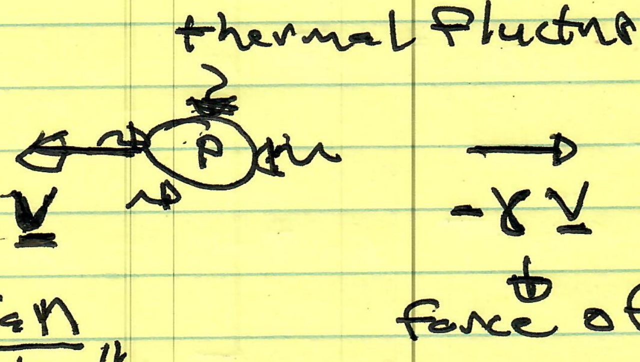
Langevin Eqn.

$$m \frac{d\underline{v}}{dt} = -\gamma \underline{v} + \underline{\tilde{f}}$$

$\lfloor T \rfloor$

η

Water, Gas



"Brownian Particle"

→ $\underline{\tilde{f}}$ is random force associated with thermal fluctuations

→ $\gamma \underline{v}$ is Stokes Drag on particle in fluid at low Re
(Radius; largest scale)

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

(η: fluid viscosity)

Some observations:

i) Linear

ii.) Additive Noise

i.e.

$$\frac{d\alpha}{dt} = -a\alpha + b\alpha^2 + \tilde{c}\,\alpha + \tilde{f}$$

Multiplicative, Additive

* Multiplicative noise is much trickier than additive noise

iii.) Local, in space and time

$$m\frac{dv}{dt} = -\gamma v + \tilde{f}(t)$$ local

$\tilde{f} \to$ random.

$\langle \tilde{f}(t)\tilde{f}(t') \rangle \to$ forcing correlation function

$\gamma \to$ local - drag independent of time history / no memory

$\boxed{\text{Markovian}}$

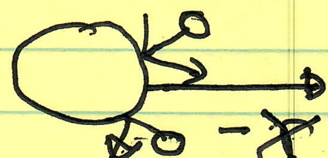
$$m \frac{dv}{dt} = -\int^{t} d\tau' \, \gamma(t-\tau) \, v(\tau) + \tilde{f}$$

non-local, memory
Drag depends on history of motion

Non-Markovian

(v.) $\tilde{f}$ → forcing Physics

$\boxed{\text{Einstein}}$
1905



$-\gamma \underline{V}$

Water Molecules ⇒ mean motion of flow, described by hydrodynamics − $\underline{V}$

+

statistical fluctuations, described as random force ⇒ i.e. discrete H_2O molecules randomly colliding w Brownian particle

− $\underline{v}'$

Water molecules play on both sides of momentum balance

→ thermal jiggling → excitation

→ collective response → damping

v.) Drag ? $\quad \gamma = 6\pi\eta R$

c.f.: "Hang time" of droplets, COVID-19.

Stokesian Hydro $\quad (\underline{\nabla}\cdot\underline{v} = 0)$

$$\rho\left(\frac{\partial \underline{v}}{\partial t} + \underline{v}\cdot\underline{\nabla}\underline{v}\right) = -\underline{\nabla}P + \eta\nabla^2\underline{v}$$

Low Re $\Rightarrow \dfrac{VL}{\nu} = \dfrac{\rho VL}{\eta} \ll 1$

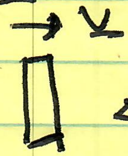
$$\left.\begin{aligned} 0 &= -\underline{\nabla}P + \eta\nabla^2\underline{v} \\ \underline{\nabla}\cdot\underline{v} &= 0 \end{aligned}\right\} \text{ Stokes Eqns.}$$

F_d on particle of radius R, $\underline{V}$

$$\underline{F_d} = -6\pi\eta R\,\underline{V}$$

Aside: Slip of paper $L_1 \times L_2$; $\underline{V}$

$Re \ll 1$



Show: ← head on

Drags some — ← knife edge.

vi.) Random

$\left\{ \begin{array}{l} \tilde{f} \text{ distributed} \\ \text{according to Gaussian} \\ \text{statistics. } (f_{eq}) \end{array} \right.$

properties

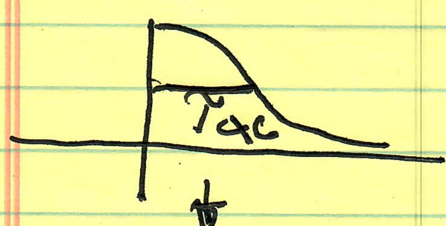
$\tilde{f}$ stationary; $\langle \tilde{f} \rangle = 0$

$\langle \tilde{f}(t_1)\tilde{f}(t_2) \rangle = \langle \tilde{f}(0)\tilde{f}(t_2 - t_1) \rangle$

$\rightarrow \langle \tilde{f}^2(0) \rangle$, $t_1 = t_2$

const. intens.

(does a characteristic scale exist)



$\tau_{ac} \rightarrow$ self correlation/coherence time

⇓

τ_{ac} short, compared any other relevant time

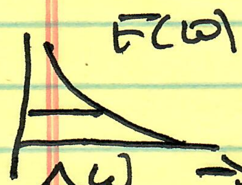
$\tau_{ac} < \gamma^{-1} < \left(\partial_t|\nabla\tilde{\phi}|^2/|\nabla\tilde{\phi}|^2\right)^{-1}$, etc.

$\langle \tilde{f}(0)\,\tilde{f}(\tau)\rangle = F(\tau)$

$\int e^{\pm i\omega\tau} F(\tau) = F(\omega)$

$\downarrow$

forcing power spectrum



$\to$ bandwidth

$\tau_{ac}\,\Delta\omega \sim 1$

<u>short τ_{ac}</u> $\to$ broad $\Delta\omega$ $\to$ "<u>white noise</u>"

White noise model useful if τ_{ac} short.

For short τ_{ac}: $\tau_{ac} \to 0$

"delta correlated"

strength

$$\langle \tilde{f}(t_1)\,\tilde{f}(t_2)\rangle = 2\,\overbrace{|\tilde{f}_0|^2}^{\uparrow}\,\tau_{ac}\,\delta(t_2 - t_1)$$

time ordering

dims!

delta correlation

$$\int d\tau \langle \tilde{f}(0)\tilde{f}(\tau)\rangle = 2|\tilde{f}|^2 \tau_{ac}$$

a) $|\tilde{v}|^2 \Rightarrow$ Fluctuation level

Now,

$$\partial_t \tilde{v} + \frac{\gamma}{m}\tilde{v} = \frac{\tilde{f}}{m}$$

$\Rightarrow$

$$\tilde{v}(t) = e^{-\frac{\gamma}{m}t}\tilde{v}(0) + \int_0^t dt' e^{-\frac{\gamma}{m}(t-t')}\frac{\tilde{f}(t')}{m}$$

so (ensemble avg.) for energy:

$$\langle \tilde{v}^2\rangle = e^{-\frac{2\gamma}{m}t}\langle \tilde{v}(0)^2\rangle$$

$$+ \langle \tilde{v}(0)\tilde{f}\rangle \text{ cross-terms}$$

$\left\{\begin{array}{l}\tilde{v}(0) \text{ i.c.}\\ \text{uncorrelated}\\ \text{with } \tilde{f}\end{array}\right.$

$$+ \int_0^t dt' \int_0^t dt'' e^{-\frac{\gamma}{m}(t-t'')} e^{-\frac{\gamma}{m}(t-t')} *$$

$$\langle \tilde{f}(t')\tilde{f}(t'')\rangle / m^2$$

but $\langle \tilde{f}(t_1)\tilde{f}(t_2)\rangle = 2|\tilde{f}_0|^2 \tau_{ac}\,\delta(t_2-t_1)$

integrating:

$$\langle \tilde{v}^2 \rangle = e^{-2\frac{\gamma}{m}t} \langle \tilde{v}(0)^2 \rangle$$

$$+ e^{-2\frac{\gamma}{m}t} \frac{2|\tilde{f}_0|^2}{m^2} \tilde{\tau}_{ac} \frac{1}{2\frac{\gamma}{m}} \left(e^{2\frac{\gamma}{m}t} - 1\right)$$

$\therefore$

$$\langle \tilde{v}^2 \rangle = \cancel{e^{-2\frac{\gamma}{m}t} \langle \tilde{v}(0)^2 \rangle}$$

$$+ \frac{\cancel{2}|\tilde{f}_0|^2 \tilde{\tau}_{ac}}{\cancel{2}\gamma m} \left(1 - \cancel{e^{-2\frac{\gamma}{m}t}}\right)$$

$t \gg \left(\frac{\gamma}{m}\right)^{-1}$ — "long time"
— long compared to $(\gamma/m)^{-1}$

$$\boxed{\langle \tilde{v}^2 \rangle = \frac{|\tilde{f}_0|^2 \tilde{\tau}_{ac}}{\gamma m}}$$

but as particle in thermal bath (fluid) at T:

$$\frac{m}{2}\langle \tilde{v}^2 \rangle = T$$

$$\Rightarrow \quad T \cong \frac{|\tilde{f}_0|^2}{2\gamma}\tilde{\tau}_{ac}$$

$$\boxed{\gamma T = \frac{|\tilde{f}_0|^2}{2}\tilde{\tau}_{ac}}$$

simple form of Fluctuation-Dissipation Theorem

i.e.

$$\boxed{\begin{gathered}\text{Noise} \sim (\text{Damping})\,T \\ \frac{\text{Noise}}{\text{Damping}} \sim T\end{gathered}}$$

Clearly here:

- "Noise" $\sim |\tilde{f}_0|^2 \tilde{\tau}_{ac}$

  Damping $\sim \gamma$

- Given any 2, deduce third

- ~ thermal equilibrium

  → emission by noise

  → absorption by damping

balance matches T!

- FDT: (as shown)

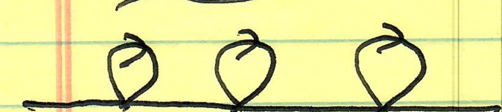
  → near equilibrium

  → linear response $(-\gamma \underline{V})$

Caveat Emptor!

⇔ beware extensions beyond regime of validity!

N.B.: Emission and Absorption at same scale $(\underline{k}, \omega)$

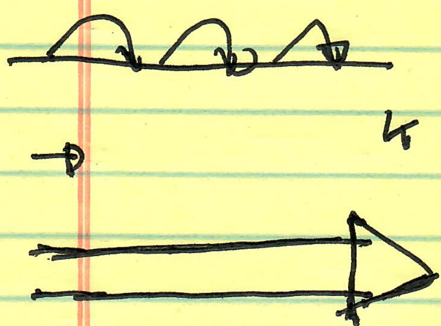


→ equilibrium fluctuation

no flux of energy on $\underline{k}, \omega$

$\boxed{\text{Quantum FDT later}}$

Contrast: Cascade — Turbulence (3D)



Energy flux
thru scales

Alternate Way $\Rightarrow$ Langevin Eqn, B.M.

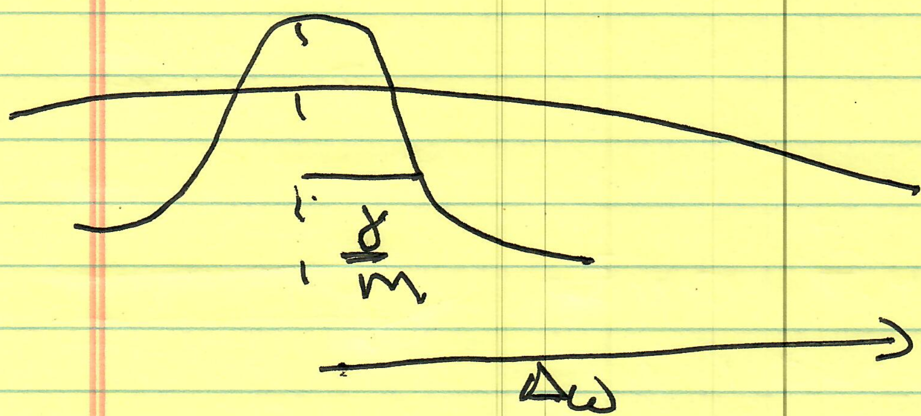
$$\partial_t \tilde{v} + \frac{\gamma}{m}\tilde{v} = \frac{\tilde{f}}{m}$$

$$-i\omega\, \tilde{v}_\omega + \frac{\gamma}{m}\tilde{v}_\omega = \frac{\tilde{f}_\omega}{m} \qquad \left\{ \begin{array}{l} \text{F. T.} \\ \text{1 pt.} \end{array} \right.$$

$$|\tilde{v}_\omega|^2 = \frac{|\tilde{f}_\omega|^2}{m^2\left(\omega^2 + (\gamma/m)^2\right)}$$

Will need integrate over ω,

so observe for white noise:



i.e. "How white is white?"

$$\Delta\omega \gg \gamma/m .$$

$\therefore$

$$\int d\omega\, |\hat{v}_\omega|^2 = \int d\omega \frac{|\tilde{f}_\omega|^2}{m^2(\omega^2 + (\gamma/m)^2)}$$

$$\cong \frac{|f_\omega|^2}{m^2} \int d\omega \frac{1}{[\omega^2 + (\gamma/m)^2]}$$

$$= \frac{|f_\omega|^2}{m^{\cancel{2}}} \frac{\cancel{m}}{\gamma} (\pi)$$

Integrating:

$$\int d\omega\, |\tilde{v}_\omega|^2 = |\tilde{v}|^2 = 2T/m$$

$$\int d\omega\, |\tilde{f}_\omega|^2 \simeq \Delta\omega\, |\tilde{f}_\omega|^2$$
$$\simeq |f_0|^2$$

$$|\tilde{f}_\omega|^2 \simeq \frac{\tau_{ac}}{\pi} |\tilde{f}_0|^2$$
$\rightarrow$ norm of F.T.!

so

$$\frac{2T}{m} \simeq \frac{|\tilde{f}_0|^2 \tau_{ac}}{m^2} \frac{m}{\gamma}$$

$\therefore$

$$\boxed{\gamma T \simeq \frac{|\tilde{f}_0|}{2} \tau_{ac}}$$

as before!

More generally:

$\hookrightarrow$ forcing / noise

$$|\tilde{v}_\omega|^2 = \frac{|\tilde{f}_\omega|^2/m^2}{|r(\omega)|^2}$$

$\hookrightarrow$ response function (susceptibility)

$$|r(\omega)|^2 \cong (\omega - \omega_{res})^2 \left|\frac{\partial r}{\partial \omega}\right|^2 + |r_{Im}|^2$$

"pole approximation" $\rightarrow$ useful, though caveat.

$\rightarrow$ response largest ~ resonance

$\rightarrow$ width set by dissipation.

example: Harmonically Bound Particle

$$\ddot{x} + \gamma \dot{x} + \omega_0^2 x = \tilde{f}/m$$

$$|\tilde{x}_\omega|^2 = \frac{|\tilde{f}_\omega|^2/m^2}{(\omega_0^2-\omega^2)^2+(\gamma\omega)^2}$$

$$\equiv \frac{|\tilde{f}_\omega|^2/m^2}{|r_{real}(\omega)|^2+|r_{IM}(\omega)|^2} \quad \text{etc.}$$

$$2\left(\tfrac{1}{2}k\langle\tilde{x}^2\rangle\right) \equiv T$$

etc.

Key's to FDT relation, Fluctuation Intensity

$\Rightarrow$ collective resonance, Dissipation $\Big\}$ susceptibility

i.e.

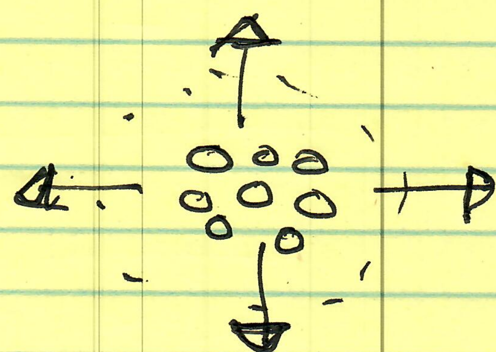
$$\nabla\cdot\underline{D} = 4\pi\rho_{ext} \Rightarrow 4\pi\rho_{fr}$$

$$D_{\substack{k\\ \omega}} = \epsilon(k,\omega)\,\underline{E}_{\substack{k\\ \omega}}$$

$\hookrightarrow$ dielectric (susceptibility)

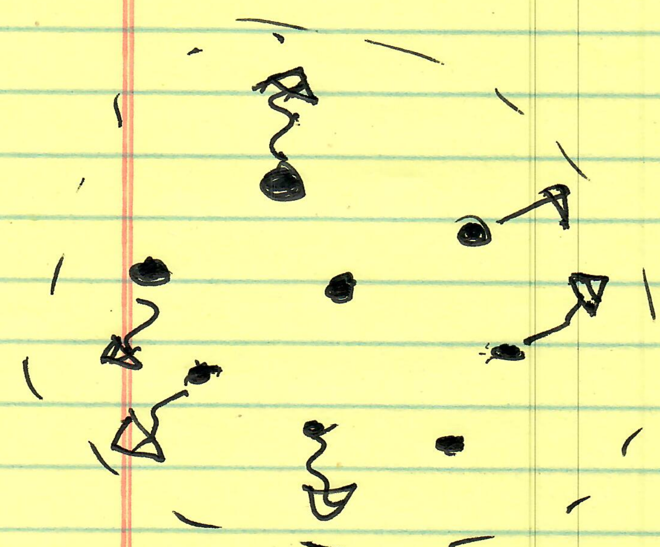
→ Now, what of position ?

Intuition:



T, η

- initial cluster of Brownian particles
- will random walk, and diffuse



so can ask, what is mean square displacement ?

so $$m \frac{\partial v}{\partial t} = -\gamma v + \tilde{f}$$

(1D, simplicity)

$t \gg (\gamma/m)^{-1}$

+ s/t "terminal velocity"

$$\frac{dx}{dt} = \frac{\tilde{f}}{\gamma}$$

simple Langevin Equation

$$x = \int_0^t dt_1 \, \frac{\tilde{f}(t_1)}{\gamma}$$

$\therefore$

$$\langle x^2 \rangle = \int_0^t dt_1 \int_0^t dt_2 \, \frac{\langle \tilde{f}(t_1)\tilde{f}(t_2) \rangle}{\gamma^2}$$

$$= \int_0^t dt_+ \int_0^\infty dt_- \, \frac{\langle \tilde{f}(0)\tilde{f}(t_-) \rangle}{\gamma^2}$$

$t_+ = (t_1 + t_2)/2$

$t_- = (t_2 - t_1)/2$

take limit to ∞, as $\langle \tilde{f}(0)\tilde{f}(t) \rangle$ cuts off beyond τ_{ac}

but $\int_0^\infty \langle \tilde{f}(0)\,\tilde{f}(t_-)\rangle\, dt_- = |\tilde{f}_0|^2\,\tilde{\tau}_{ac}$

$\Rightarrow$

$$\langle x^2 \rangle = \int^t dt\, \frac{|\tilde{f}_0|^2}{\gamma^2}\,\tilde{\tau}_{ac} = \left(\frac{|\tilde{f}_0|^2\,\tilde{\tau}_{ac}}{\gamma^2} \right) t$$

FDT: $|\tilde{f}_0|^2\,\tilde{\tau}_{ac} = 2\gamma T$

$\therefore$

$$\boxed{\langle x^2 \rangle = 2\frac{T}{\gamma}\, t \equiv 2Dt}$$

$\boxed{D = T/\gamma}$ $\rightarrow$ spatial diffusion coefficient for Brownian Motion

N.B.

$\rightarrow$ two time scales;
$\tilde{\tau}_{ac}$ – short
t – long

$\int dt_1 \int dt_2 \rightarrow t\,\tau_{ac}$.

Can say more generally:

$$x(t) = \int_0^t ds\, v(s)$$

$$\langle x^2 \rangle = \langle \int_0^t ds_1 V(s_1) \int_0^t ds_2 V(s_2) \rangle$$

$$= \int_0^t ds_1 \int_0^t ds_2 \langle V(s_1) V(s_2) \rangle$$

so

$$\frac{\partial}{\partial t} \langle x^2 \rangle = 2 \int_0^t ds \langle V(t) V(s) \rangle$$

i.e.

$$\text{above} = \int^t ds_2 \langle V(t) V(s_2) \rangle + \int_0^t ds_1 \langle V(s_1) V(t) \rangle$$

and combine

$$\partial_t \langle x^2 \rangle = 2 \int_0^t ds \langle V(t-s) V(0) \rangle$$ by stationarity

$$\equiv 2 \int_0^t du \langle V(u) V(0) \rangle$$

for $t > \tau_{ac_v}$

$$\partial_t \langle x^2 \rangle = 2\int_0^\infty du \, \langle v(u)\, v(0) \rangle$$

$$= 2D$$

$$\langle x^2 \rangle = 2Dt$$

$$\boxed{D = \int_0^\infty du \, \langle v(u)\, v(0) \rangle}$$

- D as integral of (velocity) correlation function
- (one) Kubo formula.