Lec 13 Lagrangian Mechanics / Dynamics

→ Newtonian

→ Lagrangian

→ Hamilton's

- Define a new function — called Lagrangian.

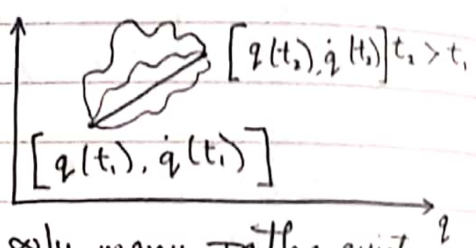
$L(q, \dot{q}; t) \quad \rightarrow \dot{q} = \frac{dq}{dt}$

generalized coordinates — generalized velocity

depends on t implicitly & not explicit
; implicit time dependence

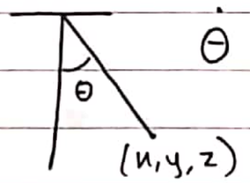
$= K(\dot{q}) - U(q)$

Kinetic energy function — Potential energy function



— ∞ly many paths exist

— which is the most probable?



$\dot{\Theta} = \frac{\partial \theta}{\partial t}$

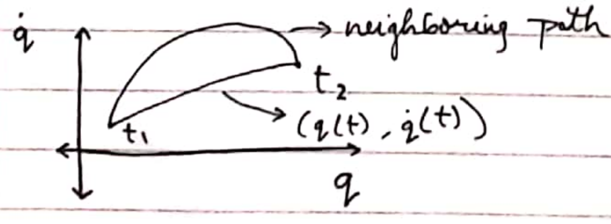
— Principle of least action

- Define action $S \equiv \int_{t_1}^{t_2} L(q, \dot{q}; t)\, dt$

Consider 2 paths:

$(q(t), \dot{q}(t)) \rightarrow$ least action path

$(q(t) + \delta q(t), \dot{q}(t) + \delta \dot{q}(t)) \rightarrow$ neighbouring path



Paths meet at t_1, t_2

$\delta q(t_1) = \delta q(t_2) = 0$

Change in S : $\int_{t_1}^{t_2} L(q + \delta q, \dot{q} + \delta \dot{q}; t)\, dt$

$- \int_{t_1}^{t_2} L(q, \dot{q}; t)\, dt = \delta S$

$= \delta \int_{t_1}^{t_2} L(q, \dot{q}; t)\, dt$

$$= \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right) dt$$

$$\delta \dot{q} = \frac{d}{dt}(\delta q)$$

$$\rightarrow \delta S = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q} \cdot \delta q + \frac{\partial L}{\partial \dot{q}} \frac{d}{dt}(\delta q) \right) dt$$

Consider the 2nd term: $\displaystyle\int_{t_1}^{t_2} \frac{\partial L}{\partial \dot{q}} \frac{d}{dt}(\delta q)\, dt$

Integrating by parts:

$$\underbrace{\left[\frac{\partial L}{\partial \dot{q}} \delta q \right]_{t_1}^{t_2}}_{=0} - \int_{t_1}^{t_2} \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}} \right) \delta q \, dt$$

$$\rightarrow \delta S = \int_{t_1}^{t_2} \frac{\partial L}{\partial q} \cdot \delta q \, dt - \int_{t_1} \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}} \right) \delta q \, dt$$

$$\rightarrow \delta S = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}} \right) \right] \delta q \, dt$$

$\rightarrow$ Since least action action $\delta S = 0$.

$\delta S = 0 \;\forall\; \delta q$

$$\Rightarrow \boxed{\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}} \right) = 0}$$ Lagrange's Equation of Motion.

Now, $\displaystyle\frac{\partial L}{\partial q} = \underbrace{-\frac{\partial U}{\partial q}}_{\text{force}}$ As $L = K(\dot{q}) - U(q)$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}} \right) \equiv \text{rate of change of generalized momentum}$$

- How do we get Hamiltonian from the lagrangian?

Calculate $\frac{dL}{dt} = \sum_{i=1}^{N} \frac{\partial L}{\partial q_i} \dot{q}_i + \sum_{i=1}^{N} \frac{\partial L}{\partial \dot{q}_i} \ddot{q}_i$

N generalized coordinates

→ from Lagrange's Equation:

$$\frac{dL}{dt} = \sum_i \dot{q}_i \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) + \sum_i \frac{\partial L}{\partial \dot{q}_i} \frac{d}{dt}(\dot{q}_i)$$

$$= \sum_i \frac{d}{dt}\left(\dot{q}_i \frac{\partial L}{\partial \dot{q}_i}\right)$$

$$\Rightarrow \frac{d}{dt}\left[\sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i}\right] - \frac{dL}{dt} = 0$$

$$\Rightarrow \frac{d}{dt}\left[\sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L\right] = 0$$

$$\Rightarrow \boxed{\sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L} \equiv \text{Constant}$$

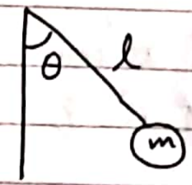
→ Hamiltonian

$$\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial K}{\partial \dot{q}_i} = m\dot{q}_i \rightarrow \sum_i \dot{q}_i (m\dot{q}_i) - L \equiv \text{Constant}$$

$$\rightarrow \boxed{K+U \equiv \text{Constant}}$$

Hamiltonian : $H \equiv K + U$

- Simple Pendulum:



Step 1: Construct L

$K(\dot{\theta}), U(\theta)$

$$L(\theta, \dot{\theta}) = K(\dot{\theta}) - U(\theta)$$

$\frac{\partial L}{\partial \theta}$ & $\frac{d}{dt}\left(\frac{\partial L}{\partial \theta}\right)$.

$$\frac{\partial L}{\partial \theta} = -mgl\sin\theta, \quad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) = ml^2\ddot{\theta}$$

$$\rightarrow m l^2 \ddot{\theta} + m g l \sin\theta = 0$$

Reference : Mechanics by Landau.

Lec 14

If L was time explicit

$$\frac{dL}{dt} = \sum_i \left[\frac{\partial L}{\partial q_i} . dq_i + \frac{\partial L}{\partial \dot{q}_i} . d\ddot{q}_i \right] + \cancel{\frac{\partial L}{\partial t}}_{0}$$

(L is not an explicit function of time, so $\frac{\partial L}{\partial t} = 0$)

$L \rightarrow$ homogeneity in time

- Homogeneity of time
  L of an isolated system does not depend on time explicitly $\rightarrow$ energy will be conserved.

– Homogeneity in time leads to energy conservation

- Conservation of momentum
  $\rightarrow$ Homogeneity of Space – the mechanical properties (would not change by any parallel displacement of the entire system.

- Displace energy particles by ϵ, velocities remaining fixed.
  $\therefore q_i \rightarrow q_i + \epsilon$. $\delta L = \sum_i \frac{\partial L}{\partial q_i} \delta q_i$

  $\therefore \delta q_i = 0$

Homogeneity of space $\Rightarrow \delta L = 0$ [Lagrangian does not change on Translation]

$$\Rightarrow \epsilon . \sum_i \frac{\partial L}{\partial q_i} = 0 \quad (\because \text{every } \delta q_i = \epsilon)$$

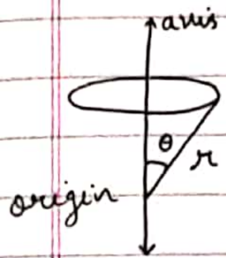
- Using Lagrange's equation:

$$\frac{d}{dt}\left[\sum_i \frac{\partial L}{\partial \dot{q}_i} \right] = 0$$

$$\Rightarrow \frac{d}{dt}\left[\sum_i mq_i\right] = 0 \Rightarrow \sum_i mq_i = \text{Constant}$$

i.e total linear momentum should be conserved.

- Conservation of Angular Momentum
  - → isotropy of space
  - → L is invariant under the rotation of the whole system by an arbitrary angle.



change in $\vec{r}$ due to rotation by $\delta\phi$ angle.

$$\delta\vec{r} = \delta\vec{\phi} \times \vec{r}$$

- $\delta\vec{\phi}$ has magnitude of $\delta\phi$ & direction along angle of rotation.

Similarly, for change in velocity:

$$\delta\vec{v} = \delta\vec{\phi} \times \vec{v}$$

$$\delta L = \sum_i \left(\frac{\partial L}{\partial \vec{r}_i} \cdot \delta\vec{r}_i + \frac{\partial L}{\partial \vec{v}_i} \cdot \delta\vec{v}_i \right)$$

Isotropy of Space : $\delta L = 0$

Use Lagrange's eqn: $\sum_i \left\{ \dot{\vec{P}}_i \cdot (\delta\vec{\phi} \times \vec{r}) + \vec{P}_i (\delta\vec{\phi} \times \vec{v}_i) \right\} = 0$

Permute factors: $(\vec{a}\,(\vec{b} \times \vec{c})) = \vec{b} \cdot (\vec{c} \times \vec{a})$
$= \vec{c} \cdot (\vec{a} \times \vec{b})$

$$\delta\vec{\phi} \cdot \sum_i (\vec{r}_i \times \dot{\vec{P}}_i + \vec{v}_i \times \vec{P}_i) = 0$$

$$\delta\vec{\phi} \cdot \frac{d}{dt}\left(\sum_i \vec{r}_i \times \vec{P}_i\right) = 0$$

Since $\delta\vec{\phi}$ is arbitrary $\rightarrow \frac{d}{dt}\left(\sum_i \vec{r}_i \times \vec{P}_i\right) = 0$

$$\Rightarrow \sum_i \{ \vec{r}_i \times \vec{P}_i \} = \text{Constant}$$

[Conservation of Angular Momentum]

– Position & Momentum are Coupled.

Lec 15 Mathematical Modelling
- Diffusion (Process)
- Random Walk (Model)

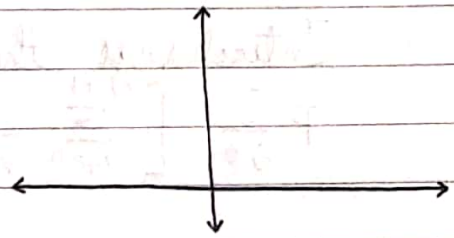
- 1D Random Walk

- A drunk starts at $x=0$
- Each step of equal length l
- Direction of each step (l or r) is random
- At each point in time, Probability to go right p, left is q.

→ P[Finding him at a certain point from origin after N steps]

- How related is this to diffusion?
  - Drop of ink added to water. Consider 1D.
  - P[finding ink molecules at a certain distance after some time t] → $P(t)$
- each ink molecule is a drunk molecule. Assumption - random walk. We have no such ink molecules.

Gaussian → as $t \uparrow$



N: total # steps
n_1: # steps to the right
n_2: # steps to the left

$N = n_1 + n_2$

Displacement m : $(n_1 - n_2) l$
l being the length of each step.

$$-Nl \le m \le Nl$$

P[n_1 out of N steps taken to the right]

$$= \frac{N!}{n_1!\, n_2!} \cdot p^{n_1} q^{n_2} = W_N(n_1)$$

Simple Case : $N=3,\ n_1=2,\ n_2=1$

$$P_N(m) = \frac{N!}{\left[\frac{N+m}{2}\right]!\,\left[\frac{N-m}{2}\right]!}\, p^{\frac{N+m}{2}} q^{\frac{N-m}{2}}$$

with $l=1$.

- Mean # steps to the right

$$\langle n_1 \rangle = \sum_{n_1=0}^{N} W_N(n_1) \cdot n_1$$

$$= \sum_{n_1=0}^{N} \frac{N!}{n_1!\,(N-n_1)!}\, p^{n_1} q^{(N-n_1)}\, n_1$$

Now, $n_1 p^{n_1} = p \frac{\partial}{\partial p} p^{n_1}$

$$\langle n_1 \rangle = \sum_{n_1=0}^{N} \frac{N!}{n_1!\,(N-n_1)!} \left[p \frac{\partial}{\partial p} p^{n_1} \right] q^{N-n_1}$$

- Interchange the order of summation & differentiation

$$p \frac{\partial}{\partial p} \left[\sum_{n_1=0}^{N} \frac{N!}{n_1\,(N-n_1)!}\, p^{n_1} q^{N-n_1} \right]$$

$$\langle n_1 \rangle = p \frac{\partial}{\partial p} (p+q)^N = pN(p+q)^{N-1}$$

$$\left.\begin{aligned} \langle n_1 \rangle &= Np \\ \langle n_2 \rangle &= Nq \end{aligned}\right\} \text{ if } p+q=1 \text{ i.e } P[\text{Not Moving}] = 0.$$

Similarly

classmate
Date
Page

- Mean Displacement
$\langle m \rangle = \langle n_1 - n_2 \rangle = \langle n_1 \rangle - \langle n_2 \rangle$

if $p = q = 1/2$, on average : $p = q$.
- electrons in a metal wire w/o bias — drunk person — same random walk model.

- Mean Squared Displacement : $\langle m^2 \rangle \neq 0$.
$\langle m^2 \rangle \neq 0$
$\langle (\Delta n_1)^2 \rangle = \langle (n_1 - \langle n_1 \rangle)^2 \rangle = \langle n_1^2 \rangle - \langle n_1 \rangle^2$

$$\langle n_1^2 \rangle = \sum_{n_1=0}^{N} \frac{N!}{n_1!\,(N-n_1)!} \cdot p^{n_1} q^{N-n_1} \; n_1^2$$

Use $n_1^2 p^{n_1} = n_1 \left(p \frac{\partial}{\partial p} p^{n_1} \right)$

$$= p \frac{\partial}{\partial p} \left(n_1 p^{n_1} \right) = p \frac{\partial}{\partial p} \left[p \frac{\partial}{\partial p} p^{n_1} \right]$$

$$\langle n_1^2 \rangle = \sum_{n_1=0}^{N} \frac{N!}{n_1!\,(N-n_1)!} \left[p \frac{\partial}{\partial p} \left(p \frac{\partial}{\partial p} p^{n_1} \right) \right] q^{N-n_1}$$

$$= p \frac{\partial}{\partial 1} \left(p \frac{\partial}{\partial p} \left\{ \sum_{n_1=0}^{N} \frac{N!}{n_1!\,(N-n_1)!} p^{n_1} q^{N-n_1} \right\} \right)$$

$$= p \frac{\partial}{\partial p} \left(p \frac{\partial}{\partial p} \{p+q\}^N \right)$$

$$= p \frac{\partial}{\partial p} \left(p \cdot N (p+q)^{N-1} \right) = p \left(N (p+q)^{N-1} + p \cdot N (N-1) (p+q)^{N-2} \right)$$

$$= p \left[N (p+q)^{N-1} + p N (N-1) (p+q)^{N-2} \right]$$
$$= p (p+q)^{N-2} \left[\cancel{Np} + Nq + pN^2 - \cancel{pN} \right]$$

$$= (pN)^2 + Npq \quad [\text{if } p+q = 1]$$
$$= \langle n_1 \rangle^2 + Npq$$

$$\langle (\Delta n_1)^2 \rangle = Npq$$

$$\langle m^2 \rangle = 4 \langle (\Delta n_1)^2 \rangle = 4 Npq$$

$p = q = 1/2$

$$\therefore \langle m^2 \rangle = 4 \langle (\Delta n_1)^2 \rangle = 4 Npq$$
$$= 4 \cdot 1/2 \cdot 1/2 \cdot N$$
$$= N$$

$$\langle m^2 \rangle = N$$

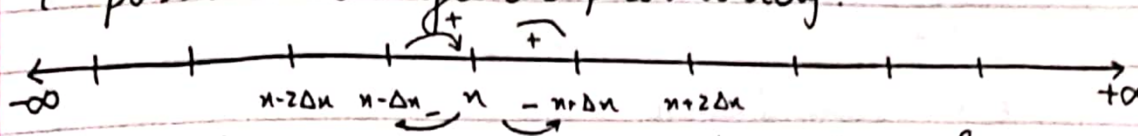
Now, $m = n_1 - n_2$
$$= 2n_1 - N$$
$$\Delta m = 2 \Delta n_1$$
$$\langle m \rangle = 2 \langle n_1 \rangle - N$$
$$\langle (\Delta m)^2 \rangle = \langle (m - \langle m \rangle)^2 \rangle = \langle m^2 \rangle$$
As $\langle m \rangle = 0$.

$$\therefore \langle (\Delta m)^2 \rangle = \langle m^2 \rangle = 4 \langle (\Delta n_1)^2 \rangle = N$$

i.e Mean Squared Displacement varies linearly with time OR #steps taken.

Lec 16 Derive Diffusion equation from Random Walk Model

4 possible changes in probability.



Δx: step length. if $\Delta x \to 0$, two space becomes continuous → diffusion.

Δt → time step. Random walker
Random walker → count velocity

$\mathbb{P}(x,t) = P$[finding random walker at x at time t]

Change in probability at x

$$\mathbb{P}(x,t+\Delta t) - \mathbb{P}(x,t) = \frac{1}{2}\mathbb{P}(x+\Delta x,t) - \frac{1}{2}\mathbb{P}(x,t) + \frac{1}{2}\mathbb{P}(x-\Delta x,t) - \frac{1}{2}\mathbb{P}(x,t)$$

$$\underbrace{\mathbb{P}(x,t+\Delta t) - \mathbb{P}(x,t)}_{\text{time variation}} = \frac{1}{2}\underbrace{\left[\mathbb{P}(x+\Delta x,t) - 2\mathbb{P}(x,t) + \mathbb{P}(x-\Delta x,t)\right]}_{\text{spatial variation}}$$

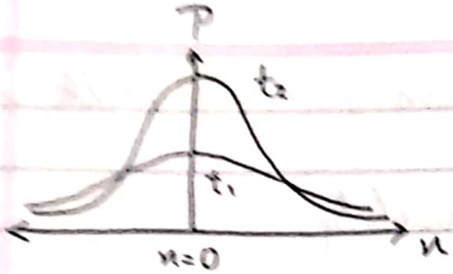
— Dividing by $(\Delta t)(\Delta x)^2$ on both sides,

$$\frac{\mathbb{P}(x,t+\Delta t) - \mathbb{P}(x,t)}{\Delta t} = \underbrace{\frac{(\Delta x)^2}{2\Delta t}}\left[\frac{\mathbb{P}(x+\Delta x,t) + \mathbb{P}(x-\Delta x,t) - 2\mathbb{P}(x,t)}{(\Delta x)^2}\right]$$

Set : $\Delta t \to 0$, $\Delta x \to 0$

$$\left\{ \frac{\partial \mathbb{P}(x,t)}{\partial t} = D \frac{\partial^2 \mathbb{P}(x,t)}{\partial x^2} \right\}$$

D → Diffusion count
↳ depends on medium
– for environmental effects



$t_2 > t_1$. P increases as a function of t.

- Prove by computation:
  after $t > 0$:
  - $\langle x \rangle = 0$
  - $\langle x^2 \rangle \propto t$

Lec 17 Recap

- diffusion
- random walk : mean displacement $\langle m \rangle = 0$

  mean squared displacement $\langle m^2 \rangle \propto N$

  $\propto t$

- diffusion equation : $\dfrac{\partial \mathbb{P}(x,t)}{\partial t} = D \dfrac{\partial^2}{\partial x^2} \mathbb{P}(x,t)$

$$\frac{\partial C(x,t)}{\partial t} = D \frac{\partial^2 C(x,t)}{\partial x^2} \qquad C: \text{concentration}$$

- One Dimensional $\mathbb{P}(x,t) \propto e^{-\frac{x^2}{4Dt}}$

- Three Dimensional $\mathbb{P}(\vec{r},t) \propto e^{-(x^2+y^2+z^2)/(4Dt)}$

: 3D diffusion equations : $\dfrac{\partial}{\partial t} \mathbb{P}(\vec{r},t)$

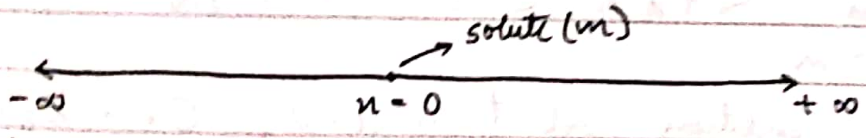
$$= D\left[\frac{\partial^2}{\partial x^2} \mathbb{P}(\vec{r},t) + \frac{\partial^2}{\partial y^2} \mathbb{P}(\vec{r},t) + \frac{\partial^2}{\partial z^2} \mathbb{P}(\vec{r},t)\right]$$

↳ isotropic diffusion.

↳ 1D : $\langle x \rangle = 0$, $\langle x^2 \rangle \propto t$

[Draw parallel with Random walk experiment]

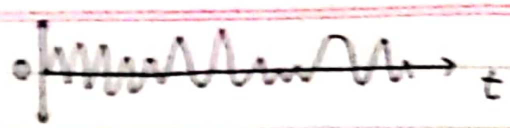
→



$\dot{x} = \dfrac{dx}{dt}$, $m \dfrac{d\dot{x}}{dt} \equiv$ damping force + random force

$$= -\alpha \dot{x} + F(t) \quad \text{—— (i)}$$

Positive Constant
(Friction Constant)

$F(t)$ 

$\langle F \rangle = 0$

(i) $\times\, x \rightarrow$

$$m x \frac{d\dot{x}}{dt} = -\alpha x \dot{x} + x F$$

$$\Rightarrow m \left[\frac{d}{dt}(x\dot{x}) - \dot{x}^2 \right] = -\alpha x\dot{x} + xF$$

— Average on both sides.

$$\Rightarrow m \left[\left\langle \frac{d}{dt}(x\dot{x}) \right\rangle - \langle \dot{x}^2 \rangle \right] = -\alpha \langle x\dot{x} \rangle + \underbrace{\langle xF \rangle}_{=0}$$

· Uncorelated Noise $\langle xF \rangle = \langle x \rangle \langle F \rangle = 0$.

— From equipartition theorem: $\frac{1}{2} m \langle \dot{x}^2 \rangle = \frac{1}{2} K_B T$

ii) $\Rightarrow m \left\langle \frac{d}{dt}(x\dot{x}) \right\rangle - K_B T = -\alpha \langle x\dot{x} \rangle$

Note: $\langle x\dot{x} \rangle = \frac{1}{2} \frac{d}{dt} \langle x^2 \rangle$

Solution: $\langle x\dot{x} \rangle = C e^{-\Gamma t} + K_B T/\alpha$

$\Gamma = \alpha/m$

Initial condition: At $t=0$, $x=0$, $C = -\dfrac{K_B T}{\alpha}$

$$\langle x^2 \rangle = \frac{2 K_B T}{\alpha} \left[t - \frac{(1-e^{-\Gamma t})}{\Gamma} \right]$$

$$\left\{ \begin{array}{l} \langle x\dot{x} \rangle = C e^{-\Gamma t} + K_B T/\alpha \\ \Rightarrow \dfrac{1}{2} \dfrac{d}{dt} \langle x^2 \rangle = C e^{-\Gamma t} + \dfrac{K_B T}{\alpha} \end{array} \right]$$ Integrate w.r.t t

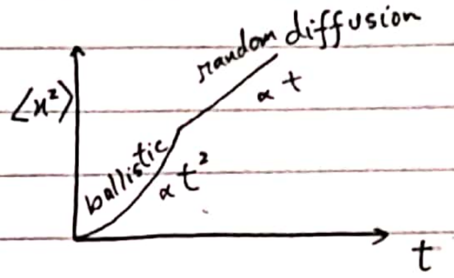
Limit 1 : $t \gg 1/\Gamma \rightarrow e^{-\Gamma t} \rightarrow 0$

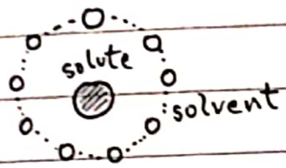
$$\langle x^2 \rangle \approx \frac{2 k_B T}{\alpha} t$$

Limit 2 : $t \ll 1/\Gamma$ (Smaller Time Scale)

$$e^{-\Gamma t} \simeq 1 - \Gamma t + 1/2\, \Gamma^2 t^2$$

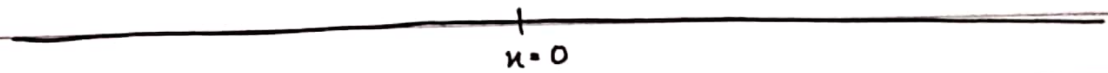
$$\langle x^2 \rangle \simeq (k_B T/m) t^2$$





- when inside : ballistic
- once outside : random

- Heat Equation.



$T(x,t)$: temperature at x at time t.

$$\frac{\partial T}{\partial t}(x,t) = D_T \frac{\partial^2 T(x,t)}{\partial x^2}$$

Thermal Diffusivity

$$D_T = \frac{\sigma_T}{\rho C}$$

σ_T = thermal conductivity

ρ = density

· Class Assignment : $\mathbb{P}(x,t) \propto e^{-\frac{x^2}{4Dt}}$

Calculate $\langle x \rangle$, $\langle x^2 \rangle$