2020-1, "STATPHYS", AULA 19

OBJETIVO: ESTUDAR A EQ. DE LANGEVIN MEDIANTE "INTEGRAÇÃO HEURÍSTICA"

ONDE ESTAMOS: 2. PROCESSOS ESTOCÁSTICOS, 2.5 PROCESSOS DE DIFUSÃO

* INTEGRAÇÃO HEURÍSTICA

→ ÚLTIMA AULA:

$$\boxed{\begin{gathered}\frac{dv}{dt} = -\gamma v + \xi(t) \\ \langle \xi(t) \rangle = 0 \; ; \; \langle \xi(t)\xi(t') \rangle = \Gamma \cdot \delta(t-t')\end{gathered}}$$

$$\begin{cases} v_{n+1} = a v_n + \sqrt{\Gamma}\sqrt{\Delta t}\, z_n \\ a = 1 - \gamma \Delta t \\ \langle z_n \rangle = 0 \; ; \; \langle z_n \cdot z_{n'} \rangle = \delta_{n,n'} \end{cases}$$

$$v_n \sim N\left(v_0 a^n, \frac{a^{2n}-1}{a^2-1}\Gamma \Delta t\right)$$

$$v(t) \sim N\left(v_0 e^{-\gamma t}, \frac{\Gamma}{2\gamma}\left(1 - e^{-2\gamma t}\right)\right)$$

→ NOVA TÉCNICA: FINJA QUE $\xi(t)$ É UMA FUNÇÃO USUAL E INTEGRE!

$$\frac{dv}{dt} = -\gamma v + \xi(t) \nearrow \begin{cases} v(t) = v_H(t) + v_P(t) \\ \dot{v}_H(t) = -\gamma v_H(t) \\ \dot{v}_P = -\gamma v_P + \xi \\ v_P(t) = c(t) . v_H(t) \end{cases}$$

$$v_H(t) = e^{-\gamma t} \; ; \; v_P(t) = e^{-\gamma t} \int_0^t dt' \xi(t') e^{\gamma t'}$$

POIS $\dot{c}(t) = \xi(t) e^{\gamma t} \Rightarrow$

$$\Rightarrow c(t) - c(t_0) = \int_{t_0}^t dt' \xi(t') e^{\gamma t'} . \quad t_0 = 0$$

ASSIM,

$$\boxed{v(t) = v_0 . e^{-\gamma t} + \int_0^t dt' \xi(t') e^{-\gamma(t-t')}} . \quad (1)$$

(i) $\langle v(t) \rangle$

$$\langle v(t) \rangle = v_0 e^{-\gamma t} + \int_0^t dt' \underbrace{\langle \xi(t') \rangle}_{=0} e^{-\gamma(t-t')}$$

$$\therefore \boxed{\langle v(t) \rangle = v_0 e^{-\gamma t}}$$

(ii) $\langle v(t_1) v(t_2) \rangle \quad t_2 > t_1$

$$\langle v(t_1)\, v(t_2) \rangle = \langle [v(t_1) - v_0 e^{-\gamma t_1}] \cdot [v(t_2) - v_0 e^{-\gamma t_2}] \rangle +$$

$$+ \cancel{v_0 e^{-\gamma t_1} \langle v(t_2) \rangle} + v_0 e^{-\gamma t_2} \langle v(t_1) \rangle -$$

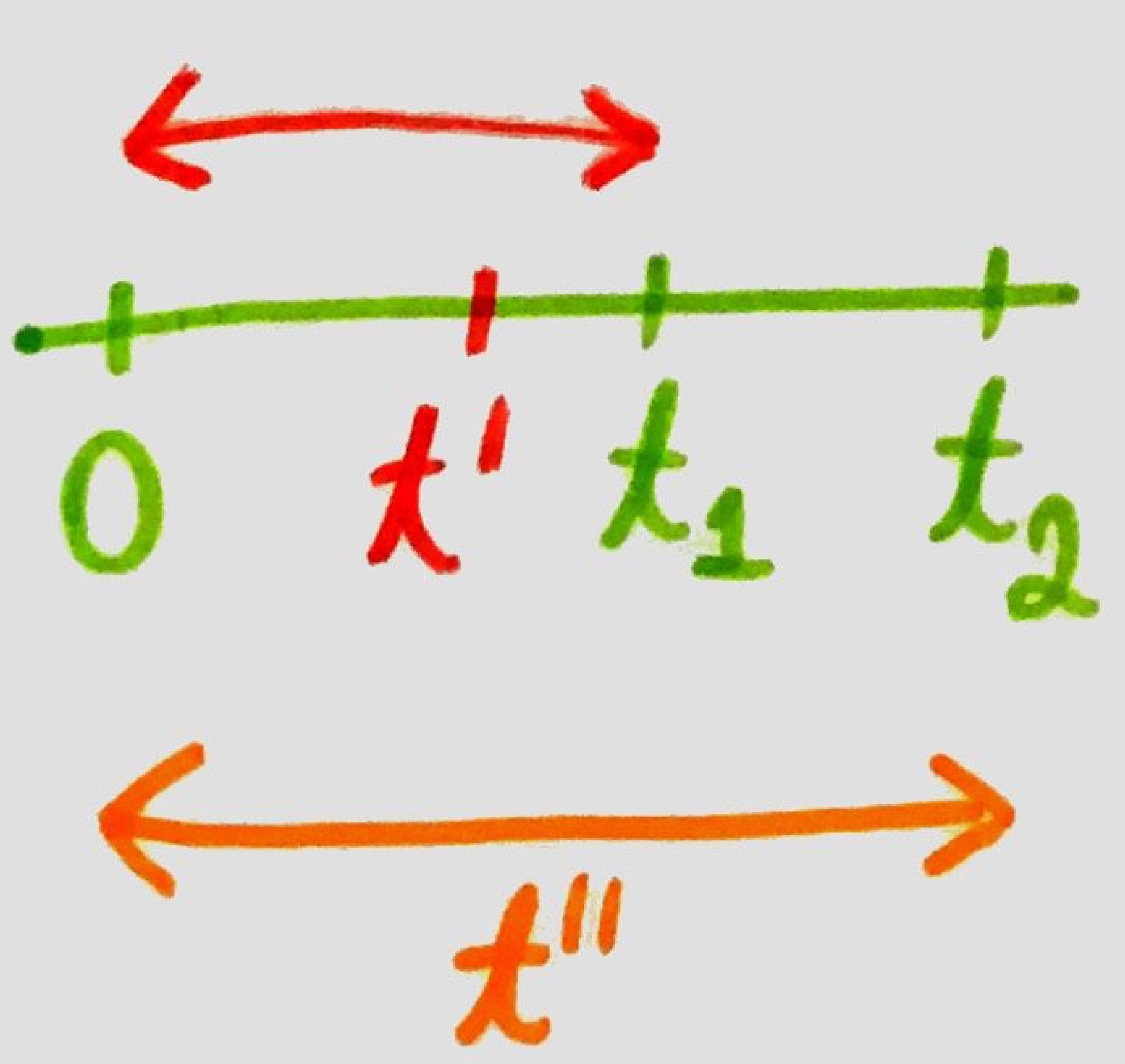
$$- \cancel{v_0^2 e^{-\gamma (t_1 + t_2)}} =$$

$$= v_0^2 e^{-\gamma (t_1 + t_2)} +$$

$$+ \left\langle e^{-\gamma t_1} \int_0^{t_1} dt' \xi(t') e^{+\gamma t'} \cdot e^{-\gamma t_2} \int_0^{t_2} dt'' \xi(t'') e^{+\gamma t''} \right\rangle =$$

$$\overset{*}{=} v_0^2 e^{-\gamma (t_1 + t_2)} +$$

$$+ e^{-\gamma (t_1 + t_2)} \int_0^{t_1} dt' e^{\gamma t'} \underbrace{\left[\int_0^{t_2} dt'' \underbrace{\langle \xi(t') \xi(t'') \rangle}_{= \Gamma . \delta(t' - t'')} e^{\gamma t''} \right]}_{= \Gamma e^{\gamma t'}} =$$



* ORDEM DE INTEGRAÇÃO MUDA TUDO!

$$= v_0^2 e^{-\gamma(t_1+t_2)} + \Gamma . e^{-\gamma(t_1+t_2)} \int_0^{t_1} dt' \, e^{2\gamma t'}$$

$$= v_0^2 e^{-\gamma(t_1+t_2)} + \Gamma e^{-\gamma(t_1+t_2)} \left(\frac{e^{2\gamma t_1} - 1}{2\gamma} \right)$$

$$\therefore \boxed{\langle v(t_1) v(t_2) \rangle = v_0^2 e^{-\gamma(t_1+t_2)} + \frac{\Gamma}{2\gamma} \left[e^{-\gamma(t_2-t_1)} - e^{-\gamma(t_2+t_1)} \right]}$$

$\downarrow$ $t_1 = t_2 = t$

$$\langle v^2(t) \rangle = v_0^2 e^{-2\gamma t} + \frac{\Gamma}{2\gamma} \left(1 - e^{-2\gamma t} \right)$$

$\downarrow$ $t \to \infty$

$$\langle v_\infty^2 \rangle = \frac{\Gamma}{2\gamma}$$

$\downarrow$ EQUIPARTIÇÃO DA ENERGIA

$$\frac{1}{2} K_B T = \frac{M \langle v_\infty^2 \rangle}{2}$$

$$\therefore \boxed{\Gamma = \frac{2\gamma K_B T}{M}}$$

*DISTRIBUIÇÕES TÉRMICAS

JÁ SABÍAMOS QUE, PARA $v_0 = 0$,

$v(t) \sim N\left(0, \frac{\Gamma}{2\gamma}\left(1 - e^{-2\gamma t}\right)\right)$. ENTÃO,

PARA $t \to \infty$, TEMOS A DISTRIBUIÇÃO DE VELOCIDADES DE MAXWELL, NO CASO UNIDIMENSIONAL:

$$\boxed{\rho(v) = \sqrt{\frac{M}{2\pi k_B T}}\, e^{-Mv^2/2k_BT}}$$

POIS $X \sim N(\mu, \sigma^2)$ É TAL QUE

$$\rho(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$, MAS $\mu = 0$

E $\sigma^2 = \frac{\Gamma}{2\gamma} = \frac{k_B T}{M}$.

→ E A <u>POSIÇÃO</u> DA PARTÍCULA BROWNIANA?

PARA $v_0 = 0$, NA DISCRETIZAÇÃO, VIMOS QUE

$$v_n = \sqrt{\Gamma}\sqrt{\Delta t}\sum_{i=0}^{n-1} a^{n-1-i}\eta_i .$$

MAS $\frac{dx}{dt} = v \rightsquigarrow x_{n+1} = x_n + \Delta t\, v_n$

$$\Downarrow$$

$$x_n = \underbrace{x_0}_{=0} + \Delta t \sum_{i=0}^{n-1} v_i$$

$$= \Delta t \sum_{i=1}^{n-1} v_i$$

$$\sum_{i=1}^{n-1}\sum_{j=0}^{i-1} a^{i-1-j}\eta_j =$$

$$= \sum_{j=0}^{n-2}\eta_j\left[\sum_{i=j+1}^{n-1} a^{i-1-j}\right] = \sum_{j=0}^{n-2}\eta_j\left[\sum_{m=0}^{n-j-2} a^m\right] =$$

$$= \sum_{j=0}^{n-2}\frac{1-a^{n-j-1}}{1-a}\eta_j$$