17/02/22

Solução de $\frac{dv}{dt} = -\gamma v + \sqrt{\Gamma}\,\xi(t)$ é

↓

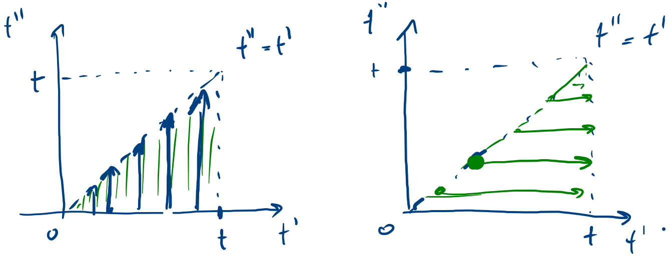
$$\boxed{v(t) = v_0 e^{-\gamma t} + e^{-\gamma t}\int_0^t e^{\gamma t'}\xi(t')\,dt'} \quad (*)$$

Vamos calcular os deslocamentos da partícula browniana.

$$\frac{dx}{dt} = v$$

$$\int_0^t \frac{dx}{dt'}\,dt' = \int_0^t v(t')\,dt'$$

$$x(t) - x_0 = \int_0^t v_0 e^{-\gamma t'}\,dt' + \int_0^t e^{-\gamma t'}\int_0^{t'} e^{\gamma t''}\xi(t'')\,dt''\,dt'$$



fazendo primeiro em t'' e depois em t'

$$\int_0^t \left(\int_0^{t'} f\,dt''\right)dt' = \int_0^t \left(\int_{t''}^t f\,dt'\right)dt''$$

$$x(t) = x_0 + \int_0^t v_0 e^{-\gamma t'}\,dt' + \int_0^t dt'' \int_{t''}^t e^{-\gamma t'} e^{\gamma t''}\xi(t'')\,dt'$$

$$= x_0 + \int_0^t v_0 e^{-\gamma t'}\,dt' + \int_0^t dt''\, e^{\gamma t''}\xi(t'')\int_{t''}^t e^{-\gamma t'}\,dt'$$

$$x(t) = x_0 + v_0\left[-\frac{e^{-\gamma t'}}{\gamma}\right]_0^t + \int_0^t dt''\left[-\frac{e^{-\gamma t'}}{\gamma}\right]_{t''}^t e^{\gamma t''}\xi(t'')$$

$$= x_0 + \frac{v_0}{\gamma}\left(1 - e^{-\gamma t}\right) + \frac{1}{\gamma}\int_0^t dt''\left(e^{-\gamma t''} - e^{-\gamma t}\right)e^{\gamma t''}\xi(t'')$$

$$\boxed{x(t) = x_0 + \frac{v_0}{\gamma}\left(1 - e^{-\gamma t}\right) + \frac{1}{\gamma}\int_0^t dt''\left[1 - e^{-\gamma(t-t'')}\right]\xi(t'')}$$

Valor mé

$$\langle x\rangle = \langle x_0\rangle + \frac{\langle v_0\rangle}{\gamma}\left(1 - e^{-\gamma t}\right) + \frac{1}{\gamma}\int_0^t dt''\left(1 - e^{A}\right)\cancel{\langle\xi(t'')\rangle}^{\,0}$$

$$\boxed{\langle x(t)\rangle = \langle x_0\rangle + \langle v_0\rangle\frac{1}{\gamma}\left(1 - e^{-\gamma t}\right)}$$

$$\begin{cases}\langle x_0\rangle = x_0\\ \langle v_0\rangle = v_0\end{cases}$$

Vamos calcular o desvio quadrático médio

$$x(t) - \langle x\rangle = \frac{1}{\gamma}\int_0^t \xi(t'')\left[1 - e^{\gamma(t''-t)}\right]dt''$$

$$\left(x(t) - \langle x\rangle\right)^2 = \left[\frac{1}{\gamma}\int_0^t \xi(t'')\left[1 - e^{\gamma(t''-t)}\right]dt''\right]\times\left[\frac{1}{\gamma}\int_0^t \xi(t')\left(1 - e^{\gamma(t'-t)}\right]dt'\right]$$

$$= \frac{1}{\gamma^2}\int_0^t\int_0^t \xi(t')\xi(t'')\left(1 - e^{\gamma(t''-t)}\right)\left(1 - e^{\gamma(t'-t)}\right)dt'\,dt''$$

Valor médio

$$\langle\left(x(t) - \langle x\rangle\right)^2\rangle = \frac{1}{\gamma^2}\int_0^t dt'\int_0^t \underbrace{\langle\xi(t')\xi(t'')\rangle}_{=\Gamma\delta(t'-t'')} \times\left[1 - e^{A}\right]\left[1 - e^{B}\right]dt''$$

$$\langle x\rangle = \langle x(t)\rangle$$

$$\langle (x(t) - \langle x \rangle)^2 \rangle = \frac{1}{\gamma^2}\int_0^t dt' \, \Gamma \left(1 - e^{\gamma(t'-t)}\right)^2$$

$t'' = t'$

$$= \frac{\Gamma}{\gamma^2}\left[\int_0^t dt' - 2e^{-\gamma t}\int_0^t dt' \, e^{\gamma t'} + e^{-2\gamma t}\int_0^t e^{2\gamma t'} dt'\right]$$

$$= \frac{\Gamma}{\gamma^2}\left\{ t - 2e^{-\gamma t}\left[\frac{1}{\gamma}e^{\gamma t} - \frac{1}{\gamma}\right] + e^{-2\gamma t}\left[\frac{e^{2\gamma t} - 1}{2\gamma}\right]\right\}$$

$$= \frac{\Gamma}{\gamma^2}\left\{ t - \frac{2}{\gamma}\left[1 - e^{-\gamma t}\right] + \frac{1}{2\gamma}\left[1 - e^{-2\gamma t}\right]\right\}$$

$$\rightarrow \langle (x(t) - \langle x \rangle)^2 \rangle = \langle x^2(t) - 2x\langle x \rangle + \langle x \rangle^2 \rangle$$

$$= \langle x^2 \rangle - 2\langle x \rangle\langle x \rangle + \langle x \rangle^2$$

$$= \langle x^2 \rangle - 2\langle x \rangle^2 + \langle x \rangle^2 = \langle x^2 \rangle - \langle x \rangle^2$$

$$\boxed{\langle x^2 \rangle - \langle x \rangle^2 = \frac{\Gamma}{\gamma^2}\left\{ t - \frac{2}{\gamma}\left[1 - e^{-\gamma t}\right] + \frac{1}{2\gamma}\left[1 - e^{-2\gamma t}\right]\right\}}$$

O que ocorre quando $t \gg 1$

$$\rightarrow \begin{cases} e^{-\gamma t} \ll 1 \\ e^{-2\gamma t} \ll 1 \end{cases}$$

Para $t \gg 1$:

$$\langle x^2 \rangle - \langle x \rangle^2 = \frac{\Gamma}{\gamma^2}\, t - \frac{2}{\gamma} + \frac{1}{2\gamma}$$

$\ll t$

$$\boxed{\langle x^2(t) \rangle - \langle x(t) \rangle^2 = \frac{\Gamma}{\gamma^2}\, t}$$

$$\Gamma = \frac{2\gamma k_B T}{m}$$

$$\langle x^2(t)\rangle - \langle x(t)\rangle^2 = \frac{2\cdot\cancel{\gamma} k_B T}{m}\frac{1}{\gamma^{\cancel{2}}}t$$

$$= \frac{2k_BT}{m\gamma}t$$

$\gamma = \frac{\alpha}{m}$ coeficiente de dissipação

$$= 2\frac{k_BT}{\alpha}t$$

$$D = \frac{k_BT}{\alpha}$$

$$\boxed{\langle x^2(t)\rangle - \langle x(t)\rangle^2 = 2Dt}$$

α de Stokes de uma esfera

$$\alpha = 6\pi\mu a$$

→ μ : viscosidade do fluido

a : raio da esfera

$$D = \frac{k_BT}{6\pi\mu a}$$

resultado de Einstein-Sutherland para o coeficiente de difusão.

$$k_B = \frac{R}{N}$$

constante de gases

N : Nº Avogadro

↳ $\underline{PV = nRT}$

$$\frac{PV}{N} = \frac{nRT}{N}$$

$$= nk_BT$$

DISCRETIZAÇÃO DA EQUAÇÃO DE LANGEVIN

$$\frac{dv}{dt} = -\gamma v + \xi(t)$$ CUIDADO!

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

$$\langle \xi(t)\xi(t') \rangle = \Gamma \delta(t-t')$$

onde $\Gamma = \dfrac{2\gamma k_B T}{m}$

$$\frac{dv}{dt} = -\gamma v + \sqrt{\frac{2\gamma k_B T}{m}}\, \xi^*(t)$$

→ Análise dimensional da eq. Langevin

MLT : Mass Length Time

$\dfrac{dv}{dt}$: aceleração ⇒ unidade $\left[\dfrac{dv}{dt}\right] = \dfrac{L}{T^2}$.

• $[-\gamma v] = \dfrac{L}{T^2}$ $\qquad [\gamma]\dfrac{L}{T} = \dfrac{L}{T^2}$

$[\gamma][v] = \dfrac{L}{T^2}$ $\qquad [\gamma] = \dfrac{1}{T}$ (frequência)

• $\left[\dfrac{2\gamma k_B T}{m}\right]^{1/2} [\xi^*] = \dfrac{L}{T^2}$

$$\frac{[\gamma]^{1/2}[k_B T]^{1/2}}{[m]^{1/2}} [\xi^*] = \frac{L}{T^2}$$

$$\underset{\text{energia}}{[k_B T]} = \underset{\text{trabalho}}{[F \Delta x]} = [m a \Delta x] = M\frac{L}{T^2}L$$

$$= \frac{ML^2}{T^2}$$

$$\left(\frac{[\gamma][k_B T]}{[m]}\right)^{1/2}[\xi^*] = \frac{L}{T^2}$$

$$\left[\frac{1}{T}\,\frac{1}{\cancel{M}}\,\frac{\cancel{M}L^2}{T^2}\right]^{1/2}[\xi^*] = \frac{L}{T^2}$$

$$\frac{\cancel{L}}{\sqrt{T}\;T}[\xi^*] = \frac{\cancel{L}}{T^2}$$

$$[\xi^*] = \frac{\sqrt{T}}{T} = \frac{1}{\sqrt{T}}$$

$$\xi^*(t) \propto \frac{1}{\sqrt{t}} \quad \leftrightarrow \text{ modelagem da delta}$$

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

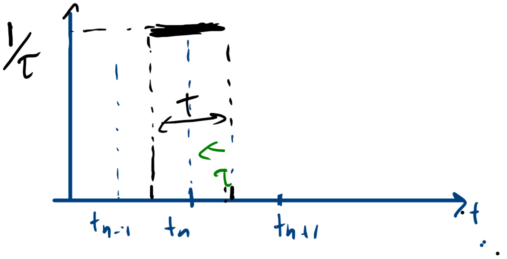
$$\langle \xi(t)\,\xi(t')\rangle = \Gamma\,\delta(t-t')$$

$$\hookrightarrow t = t' \rightarrow \langle \xi^2(t)\rangle = \Gamma\,\underbrace{\delta(0)}_{(\xi^*)^2}$$

"variância" : $\langle \xi^2(t)\rangle - \underbrace{\cancel{\langle \xi(t)\rangle}^2}_{0} = \Gamma\,\delta(0)$

→ Distribuição cuja variância é Γ multiplicada pela delta

→ Posso modelar a delta usando: $1/t$



$$t \to nT$$

$$\delta(t - t_n)$$

↳ $$\delta_n = \begin{cases} 1/\tau, & t \in [t_n - T/2 ; t_n + T/2] \\ 0, & \text{caso contrário.} \end{cases}$$

$$\int_{-\infty}^{+\infty} \delta_n(t)\, dt = \int_{t_n - T/2}^{t_n + T/2} \frac{1}{\tau}\, dt = 1$$ // ok

Contínuo:

$$\langle \xi(t)\xi(t') \rangle = \Gamma\, \delta(t - t')$$

Discreto

$$\langle \xi(nT)\, \xi(n'T) \rangle = \Gamma\, \delta_n$$

$$\langle \xi_n\, \xi_{n'} \rangle = \Gamma\, \frac{\delta_{nn'}}{\tau}.$$

onde

$$\delta_{nn'} = \begin{cases} 1, & \text{se } n = n' \\ 0, & \text{se } n \neq n' \end{cases}$$

↳ Delta de Kronecker.

* Podemos escolher ξ_n como uma gaussiana média 0 e variância $\frac{\Gamma}{\tau}$:

$$\xi_n = \sqrt{\frac{\Gamma}{\tau}}\, N(0,1),$$

onde $N(0,1)$ representa o sorteio independente de variáveis aleatórias de uma distribuição gaussiana com média 0, variância 1.

$$\rho(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$$

$\Rightarrow$ Se x é sorteado de $N(0,1)$:

$$\langle x \rangle = \int_{-\infty}^{+\infty} \underset{\text{ímpar}}{x}\, \underset{\text{par}}{\rho(x)}\, dx = 0$$

$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2 \rho(x)\, dx = 1.$$

* O que acontece com a variável $y = cx$, onde c é constante.

$$\langle cx \rangle = \int cx\, \rho(x)\, dx = c \int x\, \rho(x)\, dx = c\langle x \rangle = 0$$

$$\langle (cx)^2 \rangle = \int c^2 x^2 \rho(x)\, dx = c^2 \int x^2 \rho\, dx = \underline{c^2 \langle x^2 \rangle}$$

Discretização de

$$\frac{dv}{dt} = -\gamma v + \sqrt{\frac{2\gamma k_B T}{m}}\,\xi(t)$$

é

$$\boxed{\frac{v_{n+1} - v_n}{\tau} = -\gamma v_n + \sqrt{\frac{2\gamma k_B T}{m}}\,\overbrace{\frac{1}{\sqrt{\tau}}}^{\text{“}\sqrt{\delta}\text{”}}\,N(0,1)}$$

Teste substituindo $N(0,1)$ por outra distribuição com média 0 e variância 1

$k_B = 1$

$m = 1$

$\gamma = 2$

$\tau = 10^{-2}$

$N = 10^{3}$

$T = 0{,}8 \rightarrow \langle v^2 \rangle = \frac{k_B T}{m} = 0{,}8$

$x_0 = 0$

$v_0 = 0$