Ecuaciones de Smoluchowski para partículas activas

Francisco J Sevilla
Instituto de Física, UNAM
fjsevilla@fisica.unam.mx

25 febrero 2016

"Every theory, whether in the physical or biological or social sciences, distorts reality in that it oversimplifies. But if it is a good theory, what is omitted is outweighted by the beam of light and understanding thrown over the diverse facts."

PAUL A. SAMUELSON

Perspectives on theory at the interface of physics and biology

William Bialek
Joseph Henry Laboratories of Physics, and Lewis–Sigler Institute for Integrative Genomics, Princeton University, Princeton NJ 08544
Initiative for the Theoretical Sciences, The Graduate Center, City University of New York, 365 Fifth Ave, New York NY 10016

Theoretical physics is the search for simple and universal mathematical descriptions of the natural world. In contrast, much of modern biology is an exploration of the complexity and diversity of life. For many, this contrast is prima facie evidence that theory, in the sense that physicists use the word, is impossible in a biological context. For others, this contrast serves to highlight a grand challenge. I'm an optimist, and believe (along with many colleagues) that the time is ripe for the emergence of a more unified theoretical physics of biological systems, building on successes in thinking about particular phenomena. In this essay I try to explain the reasons for my optimism, through a combination of historical and modern examples.

I. INTRODUCTION

At present, most questions about how things w biological systems are answered by experimental ration. The situation in physics is very different, theory and experiment are more equal partners. Almost from the moment that biology and physics became sepa-

ena. What is emerging from our community goes beyond the "application" of physics to the problems of biology. We are asking physicists' questions about the phenomena of life, looking for the kinds of compelling answers that we expect in the traditional core of physics.

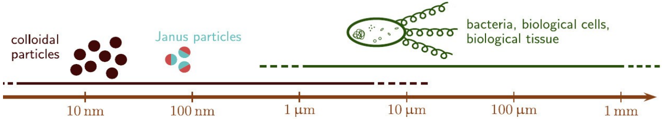
of life, looking for the kinds of compelling answers that we expect in the traditional core of physics.

Partículas Brownianas Activas

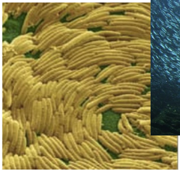
Interés en sistemas de patículas activas → Descripción estadística de sistemas alejados de estados de equilibrio (Prigogine, Haken,...)

↓

Emergencia de fenómenos colectivos asociados a grados de libertad internos

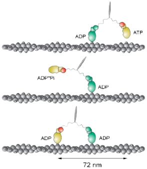


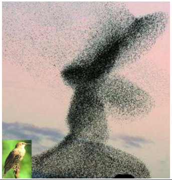
- Actividad biólogica
- Actividad en sistemas artificiales.



Ejemplos de sistemas de partículas activas

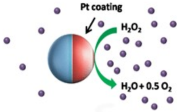
Biológicos



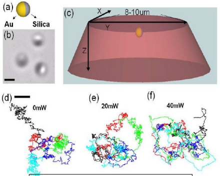


Martínez-García PRL2013
Dees Phys. Biol. 2008

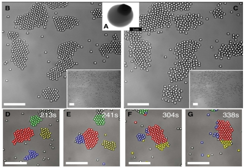
Artificiales



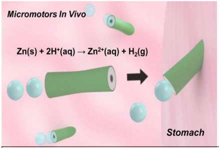
Golestanian PRL2005, NJP2007
Palacci PRL2010,Jiang PRL 2010



Palacci Science 2013



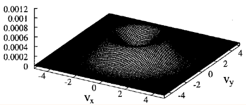
Aplicaciones

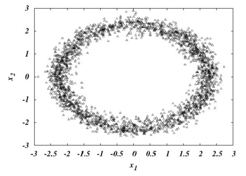


Partículas activas In Vivo
Gao ACS Nano 2014

Modelos matemáticos de movimiento activo

- Pzribram 1913, demostó que la teoría de Einstein del MB describe el movimiento de protozoarios.
- Fürth 1920, usó caminatas aleatorias persistentes para describir el movimiento de protozoarios.
- La fórmula de Fürth concide con la de Ornstein-Uhlenbeck para el promedio del cuadrado del desplazamiento.
- En el marco teórico de PBAs
- Fricción no lineal ("negative damping")- Helmholtz, Rayleigh
- "Depot models"
- Naturaleza de las fluctuaciones
- Resulta en un dinámica compleja que parece describir movimiento activo biológico
  - Propiedades difusivas novedosas de partículas activas libres
  - Distribuciones de velocidades no Gaussianas
  - Ciclos límite bajo fuerzas de confinamiento (Ebeling, Erdmann EPJ2000,PRE2002)

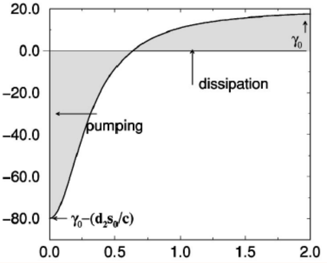


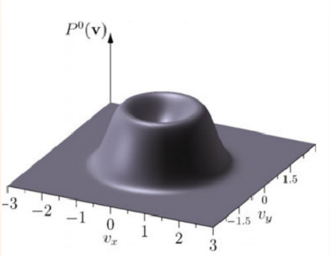


Fricción no-lineal

$$\dot{\boldsymbol{v}} = -\gamma(v)\boldsymbol{v} + \xi(t)$$

- : $\gamma(v)$
- "pumping-dissipation"
- $\gamma(v) < 0$ si $v_i < v_0$
- $\gamma(v) > 0$ si $v_i > v_0$



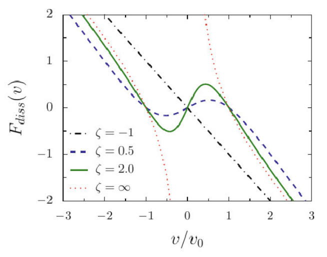


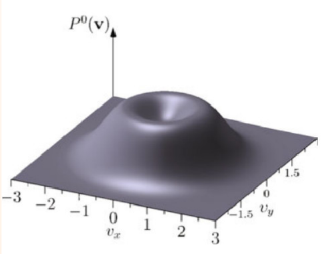
Helmholtz-Rayleigh $\gamma(v) = \gamma_0(v^2 - v_0^2)$
[ErdmannPRE2002,ErdmannEJP2000]
Schienbein-Gruler $\gamma(v) = \gamma_0(1 - v_0/v)$

- Simetría rotacional $\Rightarrow \langle \boldsymbol{v} \rangle = 0$

Fuerza disipativa $\boldsymbol{F}_{diss} = -\gamma_0 \boldsymbol{v} + d\, e(t)\boldsymbol{v}$
Dinámica del repositorio
$\dot{e} = q(\boldsymbol{r}) - ce(t) - h(\boldsymbol{v})e(t)$
$q(\boldsymbol{r}) = q_0$ y $h(\boldsymbol{v}) = d\ \boldsymbol{v}^2$

$e_{st} = q_0/(c + d\boldsymbol{v}^2)$





$$\boldsymbol{F}_{diss} = -\left[\gamma_0 - \frac{dq_0}{c+d\,\boldsymbol{v}^2}\right]\boldsymbol{v}$$

Límite de rapidez constante

$|\boldsymbol{v}| \to v_0$

Evidencia experimental: [S Bazazi,Collective motion and cannibalism in locust migratory bands 2008. H U Bdeker, Quantitative analysis of random ameboid motion. 2010. Li Dictyostelium motility as persistent random motion 2011.]]

Dinámica de peatones [Buchmueller 2007]

Purpose	v_0
Business	1.61
Leisure	1.10
Commuting	1.49
Shopping	1.16

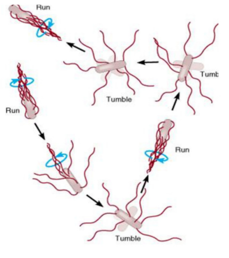
Difusión anómala: Partículas en medios heterogeneos Chepizhko PRL2013

Persistencia en sistemas de partículas bajo influencia de torcas aleatorias Radtke PRE 2012

Migración de fotones en medios dispersivos Polishchuk PRE1996, Ramakrishna IJMP2002

Movimiento activo

Run-and-tumble particles



Active Brownian particles

PRL **106,** 230601 (2011) PHYSICAL REVIEW LETTERS week ending 10 JUNE 2011

Brownian Motion with Active Fluctuations

Pawel Romanczuk[1,*] and Lutz Schimansky-Geier[1]

$$\dot{v} = -\gamma(v)v + \mathbf{e}_h \cdot \boldsymbol{\eta}(t), \qquad \dot{\varphi} = \frac{1}{v}\mathbf{e}_\varphi \cdot \boldsymbol{\eta}(t),$$

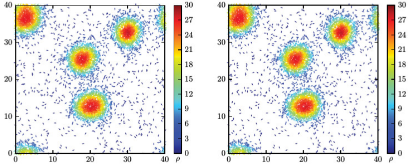
$$\boldsymbol{\eta}_a(t) = \sqrt{2D_v}\,\xi_v(t)\mathbf{e}_h + \sqrt{2D_\varphi}\,\xi_\varphi(t)\mathbf{e}_\varphi$$

EPL, **101** (2013) 20010 www.epljournal.org
doi: 10.1209/0295-5075/101/20010

When are active Brownian particles and run-and-tumble particles equivalent? Consequences for motility-induced phase separation

M. E. Cates[1] and J. Tailleur[2]

$$\dot{\psi}(\mathbf{r},\mathbf{u}) = -\nabla\cdot[v\mathbf{u}\psi(\mathbf{r},\mathbf{u})] + \nabla_{\mathbf{u}}[D_r\nabla_{\mathbf{u}}\psi(\mathbf{r},\mathbf{u})]$$
$$+\nabla(D_t\nabla\psi(\mathbf{r},\mathbf{u})) - \alpha\psi(\mathbf{r},\mathbf{u}) + \frac{\alpha}{\Omega}\int \psi(\mathbf{r},\mathbf{u}')\mathrm{d}\Omega',$$

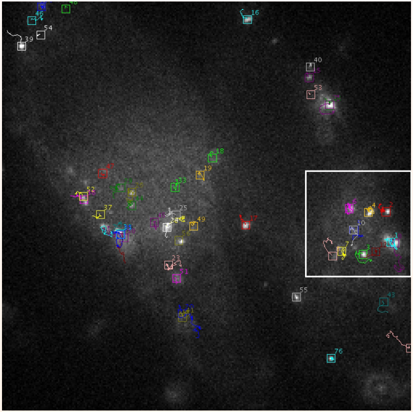


Ecuación de transporte general

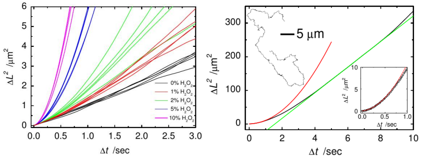
$$\frac{\partial}{\partial t}P(\boldsymbol{x},\boldsymbol{v},t)+\boldsymbol{v}\cdot\nabla P(\boldsymbol{x},\boldsymbol{v},t) = \int d^3\boldsymbol{v}'\left[K(\boldsymbol{v}|\boldsymbol{v}') - K(\boldsymbol{v}'|\boldsymbol{v})\right]P(\boldsymbol{x},\boldsymbol{v}',t)$$

Trayectorias Individuales de partículas activas

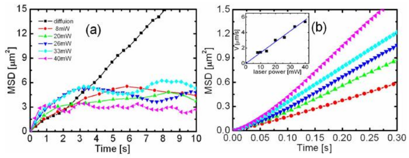
Momentos de la distribución espacial



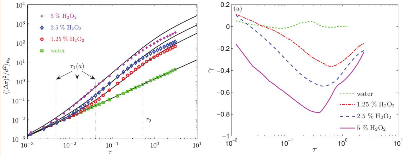
Chenouard et al. Nature Methods 2014



Howse et al. Phys. Rev. Lett. 2007



Jiang et al. Phys. Rev. Lett. 2010



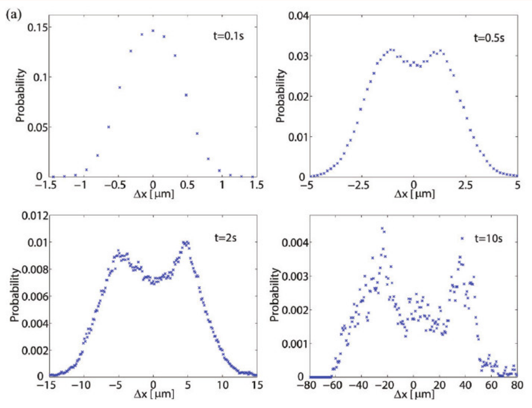
Zheng et al. Phys. Rev. E 2013

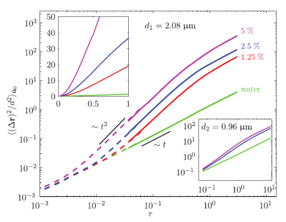
Distribución de posiciones, msd, kurtosis

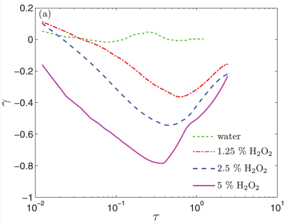
PHYSICAL REVIEW E **88**, 032304 (2013)

Non-Gaussian statistics for the motion of self-propelled Janus particles: Experiment versus theory

Xu Zheng,[1] Borge ten Hagen,[2,*] Andreas Kaiser,[2] Meiling Wu,[3] Haihang Cui,[3] Zhanhua Silber-Li,[1,†] and Hartmut Löwen[2]





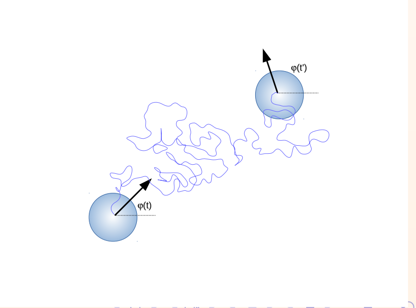


Ecuaciones de Langevin 2D

$$\frac{d}{dt}\boldsymbol{x}(t) = v_0\,\hat{\boldsymbol{v}}(t) + \boldsymbol{\xi}_T(t), \quad \frac{d}{dt}\varphi(t) = \xi_R(t).$$

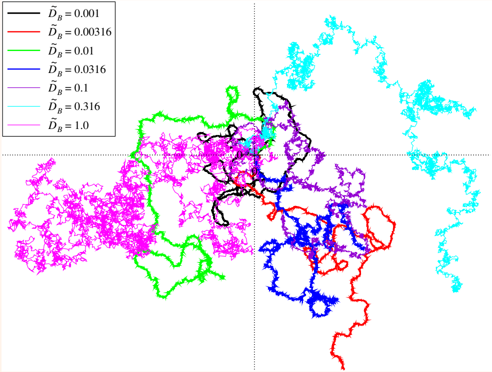
$\hat{\boldsymbol{v}} = (\cos\varphi(t), \sin\varphi(t))$
$\langle \boldsymbol{\xi}_T \rangle = \langle \xi_R \rangle = 0$
$\langle \xi_{i,T}(t)\xi_{j,T}(s)\rangle = 2D_B\delta(t-s)$; $\langle \xi_R(t)\xi_R(s)\rangle = 2D_\Omega\delta(t-s)$
$D_B = k_BT/6\pi\eta a$ coeficiente de difusión translational
D_Ω coeficiente de difusión rotational
η viscosidad del fluido

Escala de tiempo: D_Ω^{-1}
Escala de longitud: $v_0 D_\Omega^{-1}$
Inv. no. de Péclet: $\widetilde{D}_B \equiv D_B D_\Omega / v_0^2$
Partículas Janus [Pallaci PRL 2010]
$D_\Omega^{-1} \approx 0.9$ s^{-1}
$D_B \approx 0.34$ μm^2/s
$v_0 \approx 0.3 - 3.3$ μm/s
$\widetilde{D}_B \approx$ 0.035 - 4.2

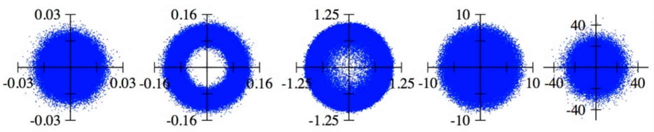


$$\frac{d}{dt}\boldsymbol{x}(t) = v_0\,\hat{\boldsymbol{v}}(t) + \boldsymbol{\xi}_T(t), \quad \frac{d}{dt}\varphi(t) = \xi_R(t).$$

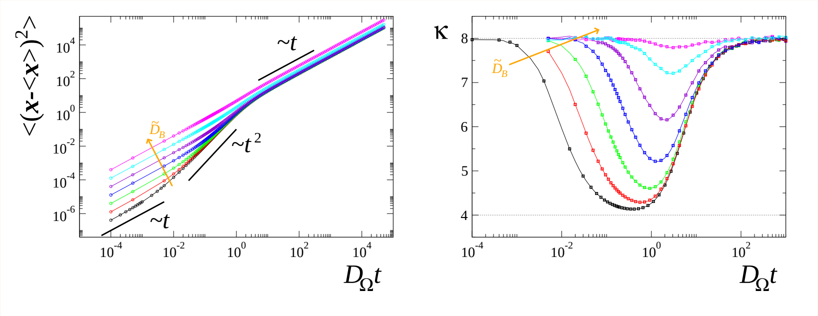
Resultados numéricos:
Esquema de integración
Euler-Cromer explícito
Paso de integración 0.001
Promedio sobre 10^5 trayectorias,
Pasos totales de integración $\times 10^6$
Condiciones iniciales: $\boldsymbol{x}_i = 0$,
$\varphi_i \in [0, 2\pi]$



Resultados numéricos



$$D_\Omega t = 0.01,\ 0.1,\ 1.0,\ 10.0,\ 100.0; \quad \widetilde{D}_B = 0.001$$



$$\widetilde{D}_B = 0.001,\ 0.00316,\ 0.01,\ 0.0316,\ 0.1,\ 0.316,\ 1.0$$

Ecuación de Fokker-Planck

$$P(\boldsymbol{x},\varphi,t) = \langle \delta(\boldsymbol{x}-\boldsymbol{x}(t))\delta(\varphi-\varphi(t))\rangle$$

$$\frac{\partial}{\partial t}P(\boldsymbol{x},\varphi,t) + v_0\hat{\boldsymbol{v}}\cdot\nabla P(\boldsymbol{x},\varphi,t) = -\frac{\partial}{\partial\varphi}\langle \xi_R(t)\delta(\boldsymbol{x}-\boldsymbol{x}(t))\delta(\varphi-\varphi(t))\rangle - \nabla\cdot\langle \boldsymbol{\xi}_T(t)\delta(\boldsymbol{x}-\boldsymbol{x}(t))\delta(\varphi-\varphi(t))\rangle,$$

Teorema Furutsu-Novikov $\langle \eta(t)F[\eta(t)]\rangle = \langle \delta F[\eta(t)]/\delta\eta(t)\rangle$

$$\frac{\partial}{\partial t}P(\boldsymbol{x},\varphi,t) + v_0\,\hat{\boldsymbol{v}}\cdot\nabla P(\boldsymbol{x},\varphi,t) = D_B\nabla^2 P(\boldsymbol{x},\varphi,t) + D_\Omega\frac{\partial^2}{\partial\varphi^2}P(\boldsymbol{x},\varphi,t).$$

$D_B = 0$: Ramakrishna 2002, FJS LA Gómez-Nava PRE 2014; $D_B \neq 0$ y confinamiento: Sandoval y Dagdug PRE 2014

Descripción reducida de partículas activas

$$P_0(\boldsymbol{x},t) = \int_0^{2\pi} d\varphi\, P(\boldsymbol{x},\varphi,t)$$

$$\widetilde{P}(\boldsymbol{k},\varphi,t) = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} \widetilde{p}_n(\boldsymbol{k},t) e^{-(D_B k^2 + D_\Omega n^2)t} e^{in\varphi},$$

$$\widetilde{p}_n(\boldsymbol{k},t) = e^{(D_B k^2 + D_\Omega n^2)t} \int_0^{2\pi} d\varphi\, \widetilde{P}(\boldsymbol{k},\varphi,t) e^{-in\varphi}.$$

$\rightarrow$ jerarquía infinita de ODEs acopladas

$$\frac{d}{dt}\widetilde{p}_n = -\frac{v_0}{2} ik\, e^{-D_\Omega t}\left[e^{2nD_\Omega t} e^{-i\theta}\, \widetilde{p}_{n-1} + e^{-2nD_\Omega t} e^{i\theta}\, \widetilde{p}_{n+1}\right].$$

donde $k_x \pm ik_y = ke^{\pm i\theta}$

Note que [FJS, Sandoval 2015]

$$P_0(\boldsymbol{x},t) = \int_0^{2\pi} d\varphi\, P(\boldsymbol{x},\varphi,t) = \boxed{(2\pi)^{-1}\int d^2k\, e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} e^{-D_B k^2 t} \widetilde{p}_0(\boldsymbol{k},t)}$$

$$P_0(\boldsymbol{x},t) = \int d^2\boldsymbol{x}'\, G(\boldsymbol{x}-\boldsymbol{x}',t)\, p_0(\boldsymbol{x}',t), \quad G(\boldsymbol{x},t) = \frac{e^{-\boldsymbol{x}^2/4D_B t}}{4\pi D_B t},$$

el propagador translacional de difusión en dos dimensiones.

Conección con la hidrodinámica fluctuante

$$\widetilde{P}(\boldsymbol{k},\varphi,t) = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty}\widetilde{p}_n(\boldsymbol{k},t)e^{-(D_B k^2 + D_\Omega n^2)t}e^{in\varphi},$$

$$\widetilde{P}(\boldsymbol{k},\varphi,t) = e^{-D_B k^2 t}\left[\widetilde{\varrho}(\boldsymbol{k},t) + e^{-D_\Omega t}\widetilde{\boldsymbol{V}}(\boldsymbol{k},t)\cdot\hat{\boldsymbol{v}} + \ e^{-2D_\Omega t}\hat{\boldsymbol{v}}\cdot\widetilde{\mathbb{W}}(\boldsymbol{k},t)\cdot\hat{\boldsymbol{v}} + \ldots\right],$$

campo escalar de densidad

$$\widetilde{\varrho}(\boldsymbol{k},t) = \frac{1}{2\pi}\widetilde{p}_0(\boldsymbol{k},t),$$

el campo vectorial $\widetilde{\boldsymbol{V}}(\boldsymbol{k},t)$

$$\widetilde{V}_x(\boldsymbol{k},t) = \frac{1}{2\pi}\left[\widetilde{p}_{-1}(\boldsymbol{k},t) + \widetilde{p}_1(\boldsymbol{k},t)\right],$$

$$\widetilde{V}_y(\boldsymbol{k},t) = \frac{i}{2\pi}\left[\widetilde{p}_1(\boldsymbol{k},t) - \widetilde{p}_{-1}(\boldsymbol{k},t)\right],$$

el campo tensorial de rango dos, simétrico y de traza cero $\widetilde{\mathbb{W}}(\boldsymbol{k},t)$

$$\widetilde{\mathbb{W}}_{xx}(\boldsymbol{k},t) = -\widetilde{\mathbb{W}}_{yy}(\boldsymbol{k},t) = \frac{1}{2\pi}\left[\widetilde{p}_2(\boldsymbol{k},t) + \widetilde{p}_{-2}(\boldsymbol{k},t)\right],$$

$$\widetilde{\mathbb{W}}_{xy}(\boldsymbol{k},t) = \widetilde{\mathbb{W}}_{yx}(\boldsymbol{k},t) = \frac{i}{2\pi}\left[\widetilde{p}_2(\boldsymbol{k},t) - \widetilde{p}_{-2}(\boldsymbol{k},t)\right]$$

$$\frac{\partial}{\partial t}\widetilde{\varrho} + \frac{v_0}{2} e^{-D_\Omega t}\, ik_i \widetilde{V}_i = 0,$$

$$\frac{\partial}{\partial t}\widetilde{V}_i + v_0 e^{D_\Omega t}\, ik_i\, \widetilde{\varrho} + \frac{v_0}{2} e^{-D_\Omega t}\, ik_j \widetilde{\mathbb{W}}_{ij} = 0,$$

$$\frac{\partial}{\partial t}\widetilde{\mathbb{W}}_{xx} + \frac{v_0}{2} e^{D_\Omega t}\ i(k_x V_x - k_y V_y) + 2D_\Omega \widetilde{\mathbb{W}}_{xx} = 0,$$

$$\frac{\partial}{\partial t}\widetilde{\mathbb{W}}_{xy} + \frac{v_0}{2} e^{D_\Omega t}\ i(k_x V_y + k_y V_x) + 2D_\Omega \widetilde{\mathbb{W}}_{xy} = 0,$$

$\partial_t \varrho(\boldsymbol{x}, t) + \nabla \cdot \boldsymbol{J}(\boldsymbol{x}, t) = 0$, $\boldsymbol{J}(\boldsymbol{x}, t)$ la transformada inversa de Fourier de $\widetilde{\boldsymbol{J}}(\boldsymbol{k}, t) = (v_0/2)e^{-D_\Omega t}\widetilde{\boldsymbol{V}}(\boldsymbol{k}, t)$.

$$\frac{\partial}{\partial t}\widetilde{V}_i(\boldsymbol{k}, t) \ + \ v_0 e^{D_\Omega t}\, ik_i\, \widetilde{\varrho}(\boldsymbol{k}, t) \ + \ \frac{v_0^2}{4} k^2 \int_0^t ds\, e^{-3D_\Omega (t-s)}\, \widetilde{V}_i(\boldsymbol{k}, s) \quad = \quad 0,$$

Soluciones explícitas para $\widetilde{\varrho}(\boldsymbol{k},\epsilon)$ y $\widetilde{\boldsymbol{V}}(\boldsymbol{k},\epsilon)$ en el dominio de Laplace,

$$\widetilde{\varrho}(\boldsymbol{k},\epsilon)=\cfrac{\widetilde{\varrho}(\boldsymbol{k},0)}{\epsilon+\cfrac{v_0^2k^2/2}{\epsilon+D_\Omega+\cfrac{v_0^2k^2/4}{\epsilon+4D_\Omega}}}$$

$$\widetilde{V}_i(\boldsymbol{k},\epsilon)=\cfrac{-ik_iv_0}{\epsilon+\cfrac{v_0^2k^2/4}{\epsilon+3D_\Omega}}\widetilde{\varrho}(\boldsymbol{k},\epsilon-D_\Omega),$$

La corriente $\widetilde{\boldsymbol{J}}(\boldsymbol{k},\epsilon)$ se obtiene de $\widetilde{\boldsymbol{J}}(\boldsymbol{k},\epsilon)=(v_0/2)\widetilde{\boldsymbol{V}}(\boldsymbol{k},\epsilon+D_\Omega)$

$$\widetilde{\boldsymbol{J}}(\boldsymbol{k},\epsilon)=-\frac{v_0^2}{2}i\boldsymbol{k}\frac{1}{\epsilon+D_\Omega+\frac{v_0^2k^2/4}{\epsilon+4D_\Omega}}\widetilde{\varrho}(\boldsymbol{k},\epsilon).$$

con lo que se concluye una relación constitutiva non-Fickiana

$$\boldsymbol{J}(\boldsymbol{x},t)=-\frac{v_0^2}{2}\nabla\int d^2\boldsymbol{y}\int_0^t ds\,\psi(\boldsymbol{x}-\boldsymbol{y},t-s)\varrho(\boldsymbol{y},s),$$

$$\widetilde{\psi}(\boldsymbol{k},t)=e^{-5D_\Omega t/2}\left[\frac{4D_\Omega}{\varpi k}\sin\varpi k+\cos\varpi_k t\right]$$

$\varpi_k^2=v_0^2k^2/2-9D_\Omega^2/4.$

Solución aproximada para $\widetilde{p}_0$

Régimen difusivo $3D_\Omega t \gg 1$

$$\frac{d}{dt}\widetilde{p}_0 = -\frac{v_0}{2} ik\, e^{-D_\Omega t}\left[e^{-i\theta}\widetilde{p}_{-1} + e^{i\theta}\widetilde{p}_1\right],$$
$$\frac{d}{dt}\widetilde{p}_{\pm 1} = -\frac{v_0}{2} ik\, \left[e^{D_\Omega t} e^{\mp i\theta}\widetilde{p}_0 + e^{-3D_\Omega t} e^{\pm i\theta}\widetilde{p}_{\pm 2}\right]$$

$$\frac{d^2}{dt^2}\widetilde{p}_0 + D_\Omega \frac{d}{dt}\widetilde{p}_0 = -\frac{v_0^2}{2} k^2 \widetilde{p}_0 - \frac{v_0^2}{4} k^2 e^{-4D_\Omega t}\left(e^{2i\theta}\widetilde{p}_2 + e^{-2i\theta}\widetilde{p}_{-2}\right).$$

$$\longrightarrow \partial_{tt} p_0(\boldsymbol{x}, t) + D_\Omega \partial_t p_0(\boldsymbol{x}, t) = \frac{v_0^2}{2}\nabla^2 p_0(\boldsymbol{x}, t)$$

Ecuación del telegrafista [Porrá et al. PRE1997]

$D_\Omega t \to \infty$, ec. de difusión, $D = v_0^2/2D_\Omega$.
$D_\Omega t \ll 1$, ec. de onda con velocidad $c = v_0/\sqrt{2}$.
Con solución en Fourier

$$\widetilde{p}_0(\boldsymbol{k}, t) = \widetilde{p}_0(\boldsymbol{k}, 0)\, e^{-D_\Omega t/2}\left[\frac{D_\Omega}{2\omega_k}\sin \omega_k t + \cos \omega_k t\right],$$

con $\omega_k^2 \equiv v_0^2 k^2/2 - D_\Omega^2/4$

Promedio del cuadrado del desplazamiento

$$\langle \boldsymbol{x}^2(t) = -\nabla^2_{\boldsymbol{k}} \left[e^{-D_B k^2 t} \widetilde{p}_0(\boldsymbol{k}, t) \right]_{\boldsymbol{k}=0}$$

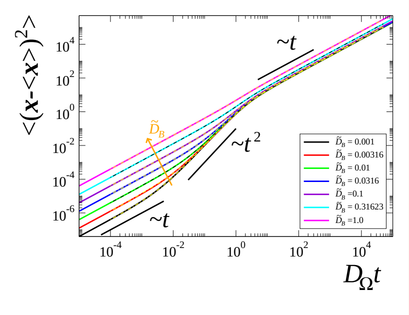
$$\langle \boldsymbol{x}^2(t) \rangle = 4 D_B t + \langle \boldsymbol{x}^2(t) \rangle_0$$

$$\frac{d^2}{dt^2} \langle \boldsymbol{x}^2(t) \rangle_0 + D_\Omega \frac{d}{dt} \langle \boldsymbol{x}^2(t) \rangle_0 =$$

$$\frac{v_0^2}{2} \left[\nabla^2_{\boldsymbol{k}} (k_x^2 + k_y^2) \widetilde{p}_0 \right]_{\boldsymbol{k}=0} + \frac{v_0^2}{4} e^{-4 D_\Omega t} \times$$

$$\left\{ \nabla^2_{\boldsymbol{k}} \left[(k_x - i k_y)^2 \widetilde{p}_{-2} + (k_x + i k_y)^2 \widetilde{p}_2 \right] \right\}_{\boldsymbol{k}=0}$$

$$\frac{d^2}{dt^2} \langle \boldsymbol{x}^2(t) \rangle_0 + D_\Omega \frac{d}{dt} \langle \boldsymbol{x}^2(t) \rangle_0 = 2 v_0^2$$



$$\langle \boldsymbol{x}^2(t) \rangle = 4 \frac{v_0^2}{D_\Omega^2} \left[\left(\widetilde{D}_B + \frac{1}{2} \right) D_\Omega t - \frac{1}{2} \left(1 - e^{-D_\Omega t} \right) \right]$$

$\widetilde{p}_0$ a tiempos más cortos

En el régimen $5D_\Omega t \gg 1,$ (modos de Fourier $n = 0, \pm 1, \pm 2$) $\longrightarrow$

$$\frac{d}{dt}\widetilde{p}_0 = -\frac{v_0}{2} e^{-D_\Omega t} \left[(ik_x + k_y)\, \widetilde{p}_{-1} + (ik_x - k_y)\, \widetilde{p}_1 \right]$$

$$\frac{d}{dt}\widetilde{p}_{\pm 1} = -\frac{v_0}{2} e^{D_\Omega t} \left[(ik_x \pm k_y)\, \widetilde{p}_0 + e^{-4D_\Omega t} (ik_x \mp k_y)\, \widetilde{p}_{\pm 2} \right]$$

$$\frac{d}{dt}\widetilde{p}_{\pm 2} = -\frac{v_0}{2} e^{3D_\Omega t} (ik_x \pm k_y)\, \widetilde{p}_{\pm 1}.$$

$$\partial_{tt} p_0(\boldsymbol{x}, t) + D_\Omega \partial_t p_0(\boldsymbol{x}, t) = v_0^2\, \nabla^2 \int_0^t ds\, \phi(t-s) p_0(\boldsymbol{x}, s) + \frac{v_0^2}{4} e^{-4D_\Omega t} Q(\boldsymbol{x})$$

Ecuación del telegrafista generalizada [FJS Gómez-Nava PRE 2014]

$\phi(t) = \frac{3}{4}\delta(t) - D_\Omega e^{-4D_\Omega t}$

$$Q(\boldsymbol{x}) = \int_0^{2\pi} d\varphi \left[e^{i2\varphi} (\partial_x + i\partial_y)^2 + e^{-i2\varphi} (\partial_x - i\partial_y)^2 - \left(\partial_x^2 + \partial_y^2\right) \right] P(\boldsymbol{x}, \varphi, 0).$$

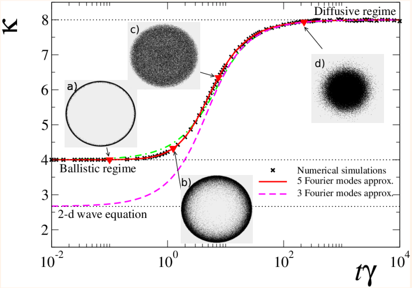
$$\widetilde{p}_0(\boldsymbol{k}, \epsilon) = \frac{(\epsilon + 4D_\Omega)(\epsilon + D_\Omega) + v_0^2 k^2/4}{(\epsilon + 4D_\Omega)\left[\epsilon^2 + D_\Omega \epsilon + (3/4) v_0^2 k^2\right] - v_0^2 D_\Omega k^2}.$$

$$\hat{P}_0(\boldsymbol{k},t) = e^{-D_B k^2 t}\hat{p}_0(\boldsymbol{k},t) \longrightarrow \hat{P}_0(\boldsymbol{k},\epsilon) = \hat{p}_0(\boldsymbol{k},\epsilon + D_B k^2)$$

La curtosis $\kappa = 4\frac{\langle \boldsymbol{x}^4(t)\rangle_r}{\langle \boldsymbol{x}^2(t)\rangle_r^2}$, $\langle \widetilde{\boldsymbol{x}^4(\epsilon)}\rangle_r = \left(\frac{1}{k}\frac{\partial}{\partial k}k\frac{\partial}{\partial k}\right)^2 \widetilde{P}_0(\boldsymbol{k},\epsilon)\Big|_{k=0}$

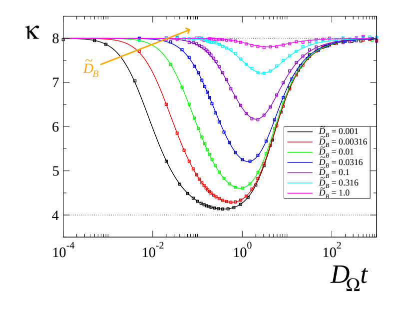
$$\langle \boldsymbol{x}^4(t)\rangle_r = 2^5\frac{v_0^4}{D_\Omega^4}\left[(D_\Omega t)^2\left(\widetilde{D}_B + \frac{1}{2}\right)^2 - \widetilde{D}_B\, D_\Omega t\left(1 - e^{-D_\Omega t}\right)\right] + \frac{v_0^4}{D_\Omega^4}\left[\frac{87}{2} - 30 D_\Omega t\left(1 + \frac{4}{9}e^{-D_\Omega t}\right) - \frac{49}{9}e^{-D_\Omega t} + \frac{1}{144}e^{-4D_\Omega t}\right].$$

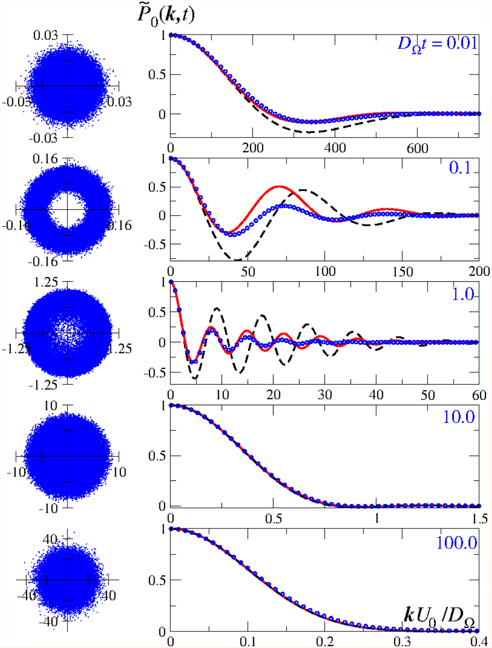
$D_B = 0$



FJS Gómez-Nava PRE 2014

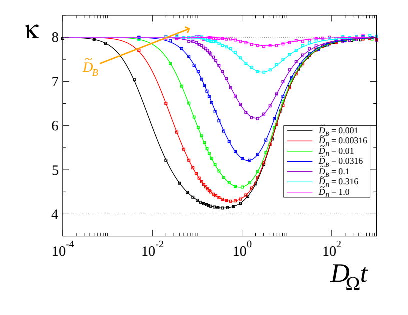
$D_B = 0.001$

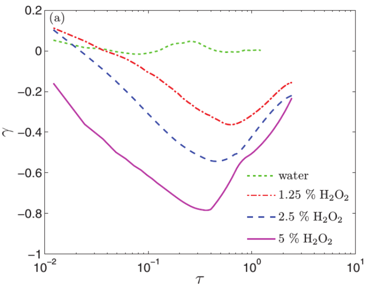



$\widetilde{P}_0(\boldsymbol{k},t)$
$D_\Omega t = 0.01$
0.1
1.0
10.0
100.0
kU_0/D_Ω

Resultados: difusión rotacional + translacional

Kurtosis (Gaussiana $\kappa = 8$)—



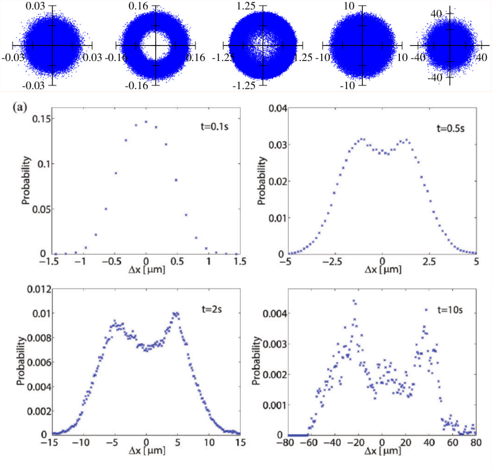


$$\kappa = \left\langle \left[(\boldsymbol{x} - \langle \boldsymbol{x} \rangle)^T \Sigma^{-1} (\boldsymbol{x} - \langle \boldsymbol{x} \rangle) \right]^2 \right\rangle$$

[FJS Sandoval 2015]

Resultados experimentales para parículas Janus, Zheng et al. PRE 2013

Resultados: difusión rotacional + translacional

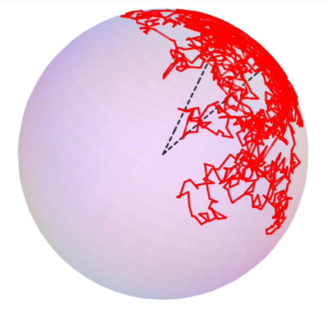


Partículas activas sujetas a torsión, caso 3D

$$\frac{d}{dt}\boldsymbol{x}(t) = v_0\,\hat{\boldsymbol{v}}(t) + \boldsymbol{\xi}_{\mathcal{T}}(t), \quad \frac{d}{dt}\hat{\boldsymbol{v}}(t) = [\boldsymbol{\tau} + \boldsymbol{\xi}_{\mathcal{R}}(t)] \times \hat{\boldsymbol{v}}(t)$$

Procesos estocásticos multiplicativos

$$\frac{d}{dt}\hat{v}_x(t) = \xi_{\mathcal{R},y}(t)\hat{v}_z(t) - \xi_{\mathcal{R},z}(t)\hat{v}_y(t)$$
$$\frac{d}{dt}\hat{v}_y(t) = \xi_{\mathcal{R},z}(t)\hat{v}_x(t) - \xi_{\mathcal{R},x}(t)\hat{v}_z(t)$$
$$\frac{d}{dt}\hat{v}_z(t) = \xi_{\mathcal{R},x}(t)\hat{v}_y(t) - \xi_{\mathcal{R},y}(t)\hat{v}_x(t)$$



$$d\theta(t) = \frac{D_\theta}{\tan\theta(t)}dt + \xi_\theta(t)dt$$
$$d\varphi(t) = \frac{\xi_\varphi(t)}{\sin\theta(t)}dt$$

Ecuación de Fokker-Planck

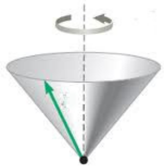
$$\frac{\partial}{\partial t}P(\boldsymbol{x},\boldsymbol{\Omega},t) + v_0\boldsymbol{\Omega}\cdot\nabla P(\boldsymbol{x},\boldsymbol{\Omega},t) = D_B\nabla^2 P(\boldsymbol{x},\hat{\boldsymbol{v}},t) +$$

$$D_\Omega\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]P(\boldsymbol{x},\hat{\boldsymbol{v}},t) +$$

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi}\left[\left(\boldsymbol{\tau}\cdot\hat{\boldsymbol{\theta}}\right)P(\boldsymbol{x},\boldsymbol{\Omega},t)\right] -$$

$$\frac{\partial}{\partial\theta}\left[\left(\boldsymbol{\tau}\cdot\hat{\boldsymbol{\varphi}}\right)P(\boldsymbol{x},\boldsymbol{\Omega},t)\right]$$

$$\boldsymbol{\Omega} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$$



$$\boldsymbol{\tau} = \tau_0\hat{\boldsymbol{z}}$$

$$\frac{\partial}{\partial t}\hat{P}(\boldsymbol{k},\boldsymbol{\Omega},t) + iv_0\boldsymbol{\Omega}\cdot\boldsymbol{k}\,\hat{P}(\boldsymbol{k},\boldsymbol{\Omega},t) = -D_B\boldsymbol{k}^2 P(\boldsymbol{k},\hat{\boldsymbol{v}},t)+$$

$$D_\Omega\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]P(\boldsymbol{k},\hat{\boldsymbol{v}},t)+$$

$$-\tau_0\frac{\partial}{\partial\varphi}P(\boldsymbol{k},\boldsymbol{\Omega},t)$$

Considere la expansión

$$\hat{P}(\boldsymbol{k},\boldsymbol{\Omega},t) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\hat{P}_n^m(\boldsymbol{k},t)e^{-[D_B k^2 + D_\Omega n(n+1) + i\tau_0 m]t}\,Y_n^m(\boldsymbol{\Omega}).$$

$Y_n^m(\boldsymbol{\Omega})$ armónicos esféricos

$$\frac{d}{dt}\hat{P}_n^m(\boldsymbol{k},t) = -iv_0 \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} \hat{P}_{n'}^{m'}(\boldsymbol{k},t)\, e^{-D_\Omega[n'(n'+1)-n(n+1)]t} e^{-i\tau_0(m'-m)t} \times$$

$$\int d\Omega\, Y_{n'}^{m'}(\boldsymbol{\Omega})[\boldsymbol{\Omega}\cdot\boldsymbol{k}]Y_n^{m*}(\boldsymbol{\Omega}),$$

Reglas de selección: $\delta_{n,n'\pm1}\delta_{m,\{m',m'\pm1\}}$

$$\frac{d}{dt}\hat{P}_n^m = \frac{v_0}{2}e^{-2D_\Omega(n+1)t}\left\{\hat{P}_{n+1}^{m+1}\left[\frac{(n+m+2)(n+m+1)}{(2n+1)(2n+3)}\right]^{1/2} e^{-i\tau_0 t}(k_y+ik_x)\right.$$
$$+\hat{P}_{n+1}^{m-1}\left[\frac{(n-m+2)(n-m+1)}{(2n+1)(2n+3)}\right]^{1/2} e^{i\tau_0 t}(k_y-ik_x)$$
$$\left.-\hat{P}_{n+1}^{m}\left[\frac{(n+m+1)(n-m+1)}{(2n+1)(2n+3)}\right]^{1/2} 2ik_z\right\}$$
$$-\frac{v_0}{2}e^{2D_\Omega nt}\left\{\hat{P}_{n-1}^{m+1}\left[\frac{(n-m)(n-m-1)}{(2n-1)(2n+1)}\right]^{1/2} e^{-i\tau_0 t}(k_y+ik_x)\right.$$
$$+\hat{P}_{n-1}^{m-1}\left[\frac{(n+m)(n+m-1)}{(2n-1)(2n+1)}\right]^{1/2} e^{i\tau_0 t}(k_y-ik_x)$$
$$\left.+\hat{P}_{n-1}^{m}\left[\frac{(n-m)(n+m)}{(2n-1)(2n+1)}\right]^{1/2} 2ik_z\right\}$$

$$\frac{d^2}{dt^2}\hat{P}_0^0(\boldsymbol{k},t) + 2D_\Omega \frac{d}{dt}\hat{P}_0^0(\boldsymbol{k},t) = -\frac{v_0^2}{3}\boldsymbol{k}^2\hat{P}_0^0(\boldsymbol{k},t) +$$

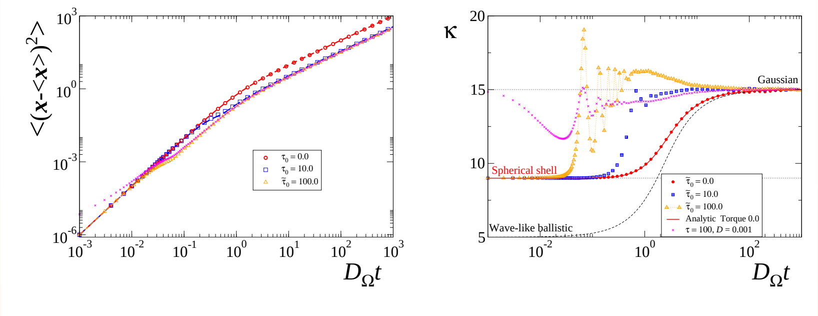
$$\left(\frac{2}{3}\right)^{1/2} i\tau_0 \frac{v_0}{2} e^{-2D_\Omega t}\left[e^{i\tau_0 t}(k_y - ik_x)\hat{P}_1^{-1} - e^{-i\tau_0 t}(k_y + ik_x)\hat{P}_1^1\right] +$$

$$\left(\frac{v_0}{2}\right)^2 e^{-6D_\Omega t}\left(\frac{8}{15}\right)^{1/2}\left[e^{-2i\tau_0 t}(k_y + ik_x)^2\hat{P}_2^2 + e^{2i\tau_0 t}(k_y - ik_x)^2\hat{P}_2^{-2}\right] -$$

$$\left(\frac{v_0}{2}\right)^2 e^{-6D_\Omega t}\left(\frac{2}{15}\right)^{1/2} 4ik_z\left[e^{-i\tau_0 t}(k_y + ik_x)\hat{P}_2^1 + e^{i\tau_0 t}(k_y - ik_x)\hat{P}_2^{-1}\right] +$$

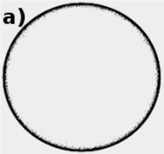
$$\left(\frac{v_0}{2}\right)^2 e^{-6D_\Omega t}\left(\frac{4}{45}\right)^{1/2} 2\left(k_x^2 + k_y^2 - 2k_z^2\right)\hat{P}_2^0$$

Si $\tau_0 = 0$:
msd: $\langle \boldsymbol{x}^2(t)\rangle = 6D_R\left[t - \frac{1}{2D_\Omega}\left(1 - e^{-2D_\Omega t}\right)\right]$
cuarto momento: $\langle \boldsymbol{x}^4(t)\rangle =$
$\frac{v_0^4}{D_\Omega^4}\left[\frac{5}{3}(D_\Omega t)^2 - \frac{26}{9}D_\Omega t - e^{-2D_\Omega t}D_\Omega t + 2\left(1 - e^{-2D_\Omega t}\right) - \frac{1}{54}\left(1 - e^{-6D_\Omega t}\right)\right]$

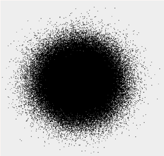


$$D_{eff} = \frac{1}{6}\frac{v_0^2}{D_\Omega}\left(\frac{1+\tau_0^2/12}{1+\tau_0^2/4}\right)$$

Generalización a D dimensiones (parte activa)



$$f_D(\boldsymbol{r}, t) = \frac{\delta(r - ct)}{A_D r^{D-1}} \Longrightarrow$$



Gaussiana

$$\frac{\partial^2 f_D(\boldsymbol{r}, t)}{\partial t^2} + \frac{1}{t}(D-1)\frac{\partial f_D(\boldsymbol{r}, t)}{\partial t} = c^2 \nabla^2 f_D(\boldsymbol{r}, t),$$

Solutions of the Spherically Symmertic Wave Equation in $p + q$ Dimensions [1]

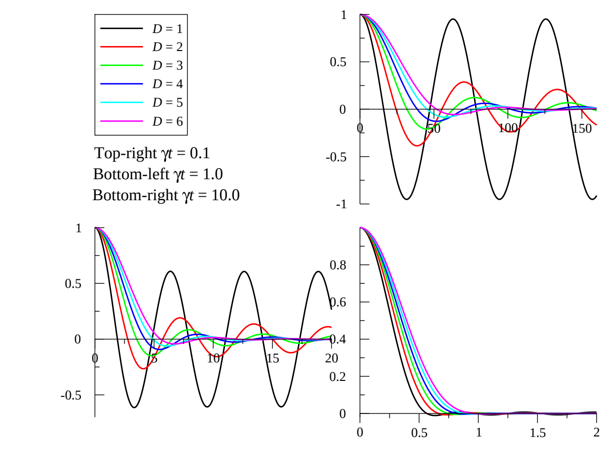
W. Bietenholz and J.J. Giambiagi
Centro Brasileiro de Pesquisas Fisicas (CBPF)
Rua Dr. Xavier Sigaud 150
22290-180 Rio de Janeiro, RJ
Brazil

3 The spherical wave equation in $p + q$ dimensions

We consider a flat space with coordinates $(t_1, \dots, t_q, x_1, \dots x_p)$ and search for solution the wave eq., which depend only on $r \doteq \sqrt{\sum_{i=1}^{p} x_i^2}$ and $\tau \doteq \sqrt{\sum_{i=1}^{q} t_i^2}$. They have to fu

$$\Big[\partial_r^2 + \frac{p-1}{r}\partial_r - \partial_\tau^2 - \frac{q-1}{\tau}\partial_\tau\Big]\phi_{p,q}(\tau, r) = 0$$

$$\frac{\partial^2 f_D(\boldsymbol{r},t)}{\partial t^2} + \left[\frac{1}{t}(D-1) + \gamma\right]\frac{\partial f_D(\boldsymbol{r},t)}{\partial t} = c^2\nabla^2 f_D(\boldsymbol{r},t),$$



$$\langle \boldsymbol{x}^2(t)\rangle = 2D\frac{c^2}{\gamma}t\left[1 - {}_2F_2(\{1,1\},\{2,D\},-\gamma t)\right].$$

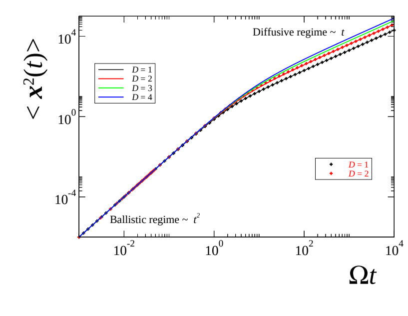
$$\langle \boldsymbol{x}^2(t)\rangle = 2d!(ct)^2\sum_{n=0}^{\infty}\frac{(-\gamma t)^n}{(n+d)!(n+2)}.$$

$\langle \boldsymbol{x}^2(t)\rangle \simeq c^2t^2 \times(1 - \frac{2}{3}\frac{\gamma t}{d+1} + \ldots),\ \gamma t \ll 1$

$\langle \boldsymbol{x}^2(t)\rangle = 2d\frac{c^2}{\gamma}t\left[1 - \frac{\gamma_e}{\gamma t} + \frac{\ln\gamma t}{\gamma t} + \ldots\right] \simeq 2d\frac{c^2}{\gamma}t,\ \gamma t \gg 1 \longrightarrow D = c^2/\gamma.$

$\gamma_e = 0.57721566490\ldots$ es la constante de Euler-Mascheroni

d	$\langle \boldsymbol{x}^2(t)\rangle$
1	$\frac{2c^2}{\gamma}\left[t - \frac{1}{\gamma}\left(1 - e^{-\gamma t}\right)\right]$
2	$\frac{4c^2}{\gamma}\left[t - \frac{1}{\gamma}\mathsf{E_{in}}\left(-\gamma t\right)\right]$
3	$\frac{6c^2}{\gamma}\left\{t - \frac{2}{\gamma}\left[\mathsf{E_{in}}\left(-\gamma t\right) - 1 + \frac{1}{\gamma t}\left(1 - e^{-\gamma t}\right)\right]\right\}$

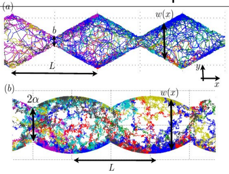


$\mathsf{E_{in}}(x) = \gamma_e + \ln x + \mathsf{E_1}(x),$

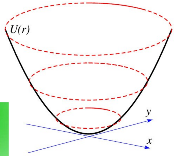
$\mathsf{E_1}(x) = \int_x^{\infty} dt\, e^{-t}/t$

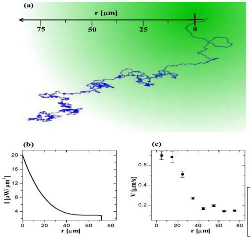
En progreso ...

Efectos de confinamiento: paredes rígidas

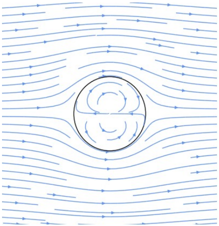


Efectos de potenciales atrapamiento





Efectos de inhomogeneidad espacial en la actividad



Efectos de flujos externos

Conclusiones y comentarios finales

- Se extendió el estudio de partículas Brownianas en alineamiento al caso de interacción de corte alcance. Diferencias "sutiles" respecto a las caracteriísticas observadas en el MV. Realizar un estudio basado en ecuaciones hidrodinámicas es necesario.
- Se extendió el método para analizar sistemáticamente las soluciones para la densidad de probabilidad marginal $P_0(\boldsymbol{x}, t)$, de la parte activa, a la situación donde las partículas también están sujetas a fluctuaciones en su traslación.
- La conección del método empleado con la descripción dada por la hidrodinámica de fluctuaciones fue exhibida explícitamente en dos dimensiones.
- Un análisis similar fue extendido al caso de tres dimensiones espaciales, en el que se consideró los efectos debidos a fuerzas externas de torsión.
- Una ecuación para la distribución de posiciones, debida a la parte activa, es propuesta fenomenólogicamente y captura cualitativamente los resultados encontrados en simulaciones numeŕicas.

Agradecimientos

- Mario Sandoval, UAM-I
- Victor Dossetti, IF-BUAP
- Alejandro Vazques Arzola IF-UNAM
- Alexandro Heiblum, University of Bristol
- Luis Aberto Gómez, Université de Nice -Sophia Antipolis

GRACIAS!