Single Active Ring Model - Supplementary Material

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1 Mean Squared Displacement for an Active Brownian Particle (ABP)

In two dimensions, a single active particle trajectory at time t is described by the its position $\vec{r}(t) = (x(t), y(t))$ and self-propelled velocity $v_0\hat{n}(t) = v_0(\cos\theta(t), \sin\theta(t))$, where $\theta(t)$ is the self-propelled velocity angle with the x-axis and v_0 is the self-propelled speed. We describe the dynamics of an isolated active Brownian by a set of overdamped Langevin equations[1–3]

$$\begin{aligned} \dot{\vec{r}}(t) &= v_0\,\hat{n}(t) + \sqrt{2D_T}\vec{\chi}(t) \ , && (1) \\ \dot{\theta}(t) &= \sqrt{2D_R}\xi(t), && (2) \end{aligned}$$

where the dot above the dynamic variables denotes temporal derivative and D_T, D_R are the thermal and rotational diffusion constants, respectively. The terms $\xi(t)$ and $\vec{\chi}(t)$ are white Gaussian noises with zero-mean, second moment $\langle\xi(t_1)\xi(t_2)\rangle = \delta(t_1 - t_2)$ and $\langle\vec{\chi}(t_1).\vec{\chi}(t_2)\rangle = 2\delta(t_1 - t_2)$. Setting the initial time $t_0 = 0$, we integrate the Langevin equations Eqs. (1), (2),

$$\begin{aligned} \vec{r}(t) &= \vec{r}_0 + v_0\int_0^t \hat{n}(t)dt + \sqrt{2D_T}\int_0^t \vec{\chi}(t)dt \ , && (3) \\ \theta(t) &= \theta_0 + \sqrt{2D_R}\int_0^t \xi(t)dt && (4) \end{aligned}$$

we recognize a Wiener process in the second term of Eq. (4). The average over different realizations in Eqs. (3), (4) results in,

$$\begin{aligned} \langle\vec{r}(t)\rangle &= \vec{r}_0 + v_0\int_0^t \langle\hat{n}(t)\rangle\, dt \ , && (5) \\ \langle\theta(t)\rangle &= \theta_0. && (6) \end{aligned}$$

The computation of second moments involves noise correlations,

$$\begin{aligned} \left\langle\vec{r}(t)^2\right\rangle &= r_0^2 + 2v_0\vec{r}_0.\int_0^t \langle\hat{n}(t)\rangle\, dt \\ &+ v_0^2\int_0^t\int_0^t \langle\hat{n}(t_1).\hat{n}(t_2)\rangle\, dt_1 dt_2 \\ &+ 2D_T\int_0^t\int_0^t \langle\vec{\chi}(t_1).\vec{\chi}(t_2)\rangle\, dt_1 dt_2 \ , && (7) \\ \left\langle\theta(t)^2\right\rangle &= \theta_0^2 + 2D_R\int_0^t\int_0^t \langle\xi(t_1)\xi(t_2)\rangle\, dt_1 dt_2, && (8) \end{aligned}$$

where we used $\langle \hat{n}(t).\vec{\chi}(t)\rangle = \langle \hat{n}(t)\rangle . \langle \vec{\chi}(t)\rangle$ and $\langle \vec{r}_0.\vec{\chi}(t)\rangle = \vec{r}_0. \langle \vec{\chi}(t)\rangle$, thus

$$\sigma^2 = \left\langle \theta(t)^2 \right\rangle - \left\langle \theta(t) \right\rangle^2 = 2D_R t. \tag{9}$$

The mean-square displacement $msd(t) = \langle (\vec{r}(t) - \vec{r}_0)^2 \rangle$ is defined by

$$\begin{aligned}
\left\langle (\vec{r}(t) - \vec{r}_0)^2 \right\rangle &= \left\langle \vec{r}(t)^2 \right\rangle + r_0^2 - 2\vec{r}_0. \langle \vec{r}(t) \rangle \ , \qquad (10)\\
\left\langle (\vec{r}(t) - \vec{r}_0)^2 \right\rangle &= v_0^2 \int_0^t \int_0^t \langle \hat{n}(t_1).\hat{n}(t_2) \rangle \, dt_1 dt_2 \\
&+ 2D_T \int_0^t \int_0^t \langle \vec{\chi}(t_1).\vec{\chi}(t_2) \rangle \, dt_1 dt_2 \ , \qquad (11)\\
\left\langle (\vec{r}(t) - \vec{r}_0)^2 \right\rangle &= v_0^2 \int_0^t \int_0^t \langle \hat{n}(t_1).\hat{n}(t_2) \rangle \, dt_1 dt_2 \\
&+ 4D_T t,
\end{aligned}$$

where the term $v_0^2 \langle \hat{n}(t_1).\hat{n}(t_2) \rangle$ is called of self-propelled velocity autocorrelation function. Since the angle $\theta(t)$ is a Wiener process, its distribution is a Gaussian with mean θ_0 and variance $\sigma^2 = 2D_R t$, thus

$$\rho(\theta(t)) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(\theta(t) - \theta_0)^2}{2\sigma^2} \right). \tag{12}$$

The mean value of self-propelled velocity direction $\langle \hat{n}(t) \rangle$ may be calculate using the angular distribution,

$$\begin{aligned}
\langle \hat{n}(t) \rangle &= \int_{-\infty}^{\infty} \rho(\theta(t))(\cos\theta(t)\hat{i} + \sin\theta(t)\hat{j}) d\theta \ , \qquad (13)\\
&= \hat{i} \int_{-\infty}^{\infty} \cos\theta(t) \rho(\theta(t)) d\theta \ ,
\end{aligned}$$

the integral in the second term of Eq. (13) is zero since the sine function is odd and the Gaussian distribution even. We can rewrite the Eq (14) as

$$\langle \hat{n}(t) \rangle = \int_{-\infty}^{\infty} \left\{ \frac{e^{i\theta} + e^{-i\theta}}{2} \right\} \rho(\theta(t)) d\theta \hat{i} \ , \tag{14}$$

$$\langle \hat{n}(t) \rangle = e^{-D_R t} \cos\theta_0 \hat{i}. \tag{15}$$

We may then calculate the self-propelled velocity autocorrelation function as follows,

$$\begin{aligned}
\langle \hat{n}(t_1).\hat{n}(t_2) \rangle &= \langle \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \rangle \ , \\
&= \langle \cos(\theta_1 - \theta_2) \rangle . \qquad (16)
\end{aligned}$$

To calculate the Eq. (16) it is necessary to know the distribution of $\bar{\theta}(\bar{t}) \equiv \theta_1 - \theta_2$, but as previously, this is a Wiener process. From Eqs. (4) and (9) we have

$$\left\langle \bar{\theta}(\bar{t}) \right\rangle = 0 \ , \tag{17}$$

$$\left\langle \bar{\theta}(\bar{t})^2 \right\rangle = 2D_R \bar{t}, \tag{18}$$

where $\bar{t} \equiv |t1 - t2|$, thus,

$$\rho(\bar{\theta}(\bar{t})) = \frac{1}{\sqrt{2\pi\sigma_{\bar{\theta}}^2}} \exp\left(-\frac{\bar{\theta}(\bar{t})^2}{2\sigma_{\bar{\theta}}^2} \right), \tag{19}$$

where $\sigma_{\bar{\theta}}^2 = 2D_R\bar{t}$. Using the same procedure of Eq. (14), but with $\cos\bar{\theta}$ and $\rho(\bar{\theta}(\bar{t}))$, we obtain

$$\langle \hat{n}(t_1).\hat{n}(t_2)\rangle = \int_{-\infty}^{\infty}\left\{\frac{e^{i\bar{\theta}}+e^{-i\bar{\theta}}}{2}\right\}\rho(\bar{\theta}(t))d\bar{\theta}\ , \tag{20}$$

$$\langle \hat{n}(t_1).\hat{n}(t_2)\rangle = e^{-D_R|t_1-t_2|}. \tag{21}$$

To write the $msd(t)$ we use Eqs. (11) and (21),

$$\begin{aligned} v_0^2\int_0^t\int_0^t e^{-D_R|t_1-t_2|}dt_1dt_2 &= v_0^2\int_0^t\int_0^{t_1} e^{D_R(t_2-t_1)}dt_2dt_1 \\ &+ v_0^2\int_0^t\int_0^{t_2} e^{D_R(t_1-t_2)}dt_1dt_2, \\ &= \frac{v_0^2}{D_R}\int_0^t(1-e^{-D_Rt_1})dt_1 \\ &+ \frac{v_0^2}{D_R}\int_0^t(1-e^{-D_Rt_2})dt_2, \end{aligned}$$

$$msd(t) = 4D_Tt + \frac{2v_0^2}{D_R}\left[t+\frac{1}{D_R}(e^{-D_Rt}-1)\right], \tag{22}$$

$$msd(t) = 4D_Tt + 2l_p^2\left[\frac{t}{\tau_R}+(e^{-t/\tau_R}-1)\right], \tag{23}$$

where $l_p = v_0\tau_R$ is the persistence length and $\tau_R = 1/D_R$ is called persistence time. At short times, $t \ll 4D_T/v_0^2$, the motion is diffusive with the typical Brownian short-time thermal constant diffusion, $msd(t) = 4D_Tt$. At intermediate times, $4D_T/v_0^2 < t < 1/D_R$, the motion is ballistic, and we find $msd(t) = 4D_Tt+v_0^2t^2$. At long times $t \gg 1/D_R$, the motion is diffusive com $msd(t) = 4D_Tt+2v_0^2t/D_R = 4Dt$, where $D = D_T + v_0^2/2D_R$ is the diffusion coefficient constant.

2 Mean Square Displacement for a System of Active Brownian Particles $\tau \to \infty$

For a system with N interacting active Brownian particles, the center of mass position dynamics $\vec{R}_{CM}(t)$ follows equation

$$\dot{\vec{R}}_{CM}(t) = \frac{v_0}{N}\sum_i^N \hat{n}_i(t) + \frac{\mu}{N}\sum_i^N\sum_{i\sim j}\nabla U(\vec{r}_i(t)) + \frac{\sqrt{2D_R}}{N}\sum_i^N \vec{\chi}_i(t), \tag{24}$$

where the self orientation of each particle is given by

$$\dot{\theta}_i(t) = \sqrt{2D_R}\xi_i(t), \tag{25}$$

being $\xi_i(t)$ and $\vec{\chi}_i(t)$ Gaussian white noises with zero-mean with second moment $\langle\xi_i(t_1)\xi_j(t_2)\rangle = \delta_{ij}\delta(t_1-t_2)$ and $\langle\vec{\chi}_i(t_1).\vec{\chi}_j(t_2)\rangle = 4D_T\delta_{ij}\delta(t_1-t_2)$ independently for each particle at each time-step. Since all forces derived from the potential are internal, Eq. (24) reduces to

$$\dot{\vec{R}}_{CM}(t) = \frac{v_0}{N}\sum_{i}^{N}\hat{n}_i(t) + \frac{\sqrt{2D_R}}{N}\sum_{i}^{N}\vec{\chi}_i(t), \tag{26}$$

Therefore, using the same procedure of the previous section, defining $MSD(t) = \left\langle (\vec{R}_{CM}(t) - \vec{R}_{CM}(0))^2 \right\rangle$, we find,

$$\begin{aligned} MSD(t) &= \frac{1}{N^2}\sum_{i}^{N}\sum_{j}^{N}\{\ v_0^2\int_0^t\int_0^t \langle \hat{n}_i(t_1).\hat{n}_j(t_2)\rangle\, dt_1 dt_2 \\ &+ 2D_T\int_0^t\int_0^t \langle \vec{\chi}_i(t_1).\vec{\chi}_j(t_2)\rangle\, dt_1 dt_2\ \}, \end{aligned} \tag{27}$$

where

$$\langle \hat{n}_i(t)\rangle = e^{-D_R t}\cos\theta_0 \hat{i}\ , \tag{28}$$

$$\langle \hat{n}_i(t_1).\hat{n}_j(t_2)\rangle = \delta_{ij}e^{-D_R|t_1-t_2|}. \tag{29}$$

Using Eq. (29) in Eq. (27), we get

$$\begin{aligned} MSD(t) &= \frac{1}{N}\{\ v_0^2\int_0^t\int_0^t e^{-D_R|t_1-t_2|}dt_1 dt_2 \\ &+ 4D_T\int_0^t\int_0^t \delta(t_1-t_2)dt_1 dt_2\ \}, \end{aligned} \tag{30}$$

$$MSD(t) = \frac{msd(t)}{N}, \tag{31}$$

$$MSD(t) = \frac{4D_T}{N}t + \frac{2v_0^2}{D_R N}\left[t + \frac{1}{D_R}(e^{-D_R t} - 1)\right], \tag{32}$$

$$MSD(t) = \frac{4D_T}{N}t + 2L_p^2\left[\frac{t}{\tau_R} + (e^{-D_R t} - 1)\right], \tag{33}$$

where $L_p = v_0\tau_R/\sqrt{N}$ is the persistence length. We can analyze the center of mass velocity fluctuations using Eq. (26),

$$\begin{aligned} \dot{\vec{R}}_{CM}(t) &= \frac{v_0}{N}\sum_{i}^{N}\hat{n}_i(t) + \frac{\sqrt{2D_R}}{N}\sum_{i}^{N}\vec{\chi}_i(t), \\ \vec{V}_{CM}(t) &= \frac{v_0}{N}\sum_{i}^{N}\hat{n}_i(t) + \frac{\sqrt{2D_R}}{N}\sum_{i}^{N}\vec{\chi}_i(t), \end{aligned} \tag{34}$$

$$\begin{aligned} \left\langle \vec{V}_{CM}(t)\right\rangle &= \frac{v_0}{N}\sum_{i}^{N}\langle \hat{n}_i(t)\rangle = v_0 e^{-D_R t}\cos\theta_0\hat{i}, \\ \left\langle \vec{V}_{CM}(t)\right\rangle^2 &= v_0^2 e^{-2D_R t}\cos^2\theta_0 \xrightarrow{t\gg 1} 0. \end{aligned} \tag{35}$$

The second moment of $\vec{V}_{CM}(t)$ is

$$\left\langle \vec{V}_{CM}^2(t) \right\rangle = \frac{v_0^2}{N^2} \sum_i^N \sum_j^N \langle \hat{n}_i(t).\hat{n}_j(t) \rangle , \tag{36}$$

where we use $\langle \hat{n}_i(t).\vec{\chi}_j(t)\rangle = \langle \hat{n}_i(t)\rangle . \langle \vec{\chi}_j(t)\rangle$ and $\langle \vec{\chi}_i(t).\vec{\chi}_j(t)\rangle = \langle \vec{\chi}_i(t)\rangle . \langle \vec{\chi}_j(t)\rangle$. Using the Eq. (29) in Eq. (36) we get

$$\left\langle \vec{V}_{CM}^2(t) \right\rangle = \frac{v_0^2}{N}. \tag{37}$$

Substituting Eq. (37) in Eq. (32), we obtain

$$MSD(t) = \frac{4D_T}{N} t + 2 \left\langle \vec{V}_{CM}^2(t) \tau_R \right\rangle \left[t + \tau_R (e^{-t/\tau_R} - 1) \right]. \tag{38}$$

3 Order parameter fluctuation

From Eq. (37) we obtain the stationary fluctuation of $\vec{V}_{CM}^2$ for a system of ABP's,

$$\delta \vec{V}_{CM}^2 = \left\langle \vec{V}_{CM}^2 \right\rangle - \left\langle \vec{V}_{CM} \right\rangle^2 = \frac{v_0^2}{N}, \tag{39}$$

the definition of the translational order parameter is

$$\varphi(t) = \frac{1}{N} \left| \sum_i^N \frac{\vec{v}_i(t)}{|\vec{v}_i(t)|} \right| ,$$

since forces in the ring are internal, we may approach $|v_i| \sim |v_0 + \delta v_i|$ and rewrite Eq. (39) in first order approach as

$$\varphi(t) \sim \frac{1}{N v_0} \left| \sum_i^N \vec{v}_i(t) \right| , \tag{40}$$

while for the CM velocity we have,

$$\vec{V}_{CM}^2(t) = \left| \vec{V}_{CM}(t) \right|^2 = \frac{1}{N^2} \left| \sum_i^N \vec{v}_i(t) \right|^2 , \tag{41}$$

comparing Eqs. (39), (40) and (41), we conclude that

$$\delta\varphi(t)^2 = \left\langle \varphi(t)^2 \right\rangle - \left\langle \varphi(t) \right\rangle^2 \sim \frac{1}{N}, \tag{42}$$

$$\delta\varphi(t) = \sqrt{\langle \varphi(t)^2 \rangle - \langle \varphi(t) \rangle^2} \sim \frac{1}{\sqrt{N}}. \tag{43}$$

4 Ratio between radius of gyration of a rod and a circumference

The radius of gyration is defined as

$$
\begin{aligned}
R_{xx}(t) &= \frac{1}{N}\sum_{i}^{N}(x_i(t) - X_{cm}(t))^2, &(44)\\
R_{yy}(t) &= \frac{1}{N}\sum_{i}^{N}(y_i(t) - Y_{cm}(t))^2, &(45)\\
R_g(t)^2 &= R_{xx}(t) + R_{yy}(t). &(46)
\end{aligned}
$$

when the active ring is in circular format with radius R, its radius of gyration is

$$
R^2_{g,cir} = R^2 = \left(\frac{Nr_0}{2\pi}\right)^2, \qquad (47)
$$

r_0 being the distance between the particles composing the ring. In the limit the ring becomes a rod we can approach it by two parallel chains with $N/2$ particles (Fig. 1) and we may calculate R_{xx} and R_{yy} as follows

$$
\begin{aligned}
R_{xx} &= \frac{4}{N}\sum_{k=1}^{\frac{N-1}{4}}(kr_0)^2,\\
R_{xx} &= \frac{r_0^2}{48N}(N-1)(N+1)(N+3),\\
R_{xx} &= \frac{r_0^2}{48}\left(N^2 + 3N - \frac{3}{N} - 1\right). &(48)\\
R_{yy} &= \frac{1}{N}\sum_{k=1}^{N}\left(\frac{r_0}{2}\right)^2,\\
R_{yy} &= \frac{r_0^2}{4}. &(49)
\end{aligned}
$$

Thus, we got $R^2_{g,rod}$

$$
\begin{aligned}
R^2_{g,rod} &= R_{xx} + R_{yy},\\
R^2_{g,rod} &= \frac{r_0^2}{48}\left(N^2 + 3N - \frac{3}{N} + 11\right), &(50)
\end{aligned}
$$

Through of Eq. (47) and Eq. (50) we got the ratio

$$
\frac{R_{g,rod}}{R_{g,cir}} = \sqrt{\frac{4\pi^2}{48}\left(1 + \frac{3}{N} + \frac{11}{N^2} - \frac{3}{N^3}\right)}. \qquad (51)
$$

When $N \gg 1$

$$
\frac{R_{g,rod}}{R_{g,cir}} = \frac{\pi}{2\sqrt{3}} = 0.90689. \qquad (52)
$$

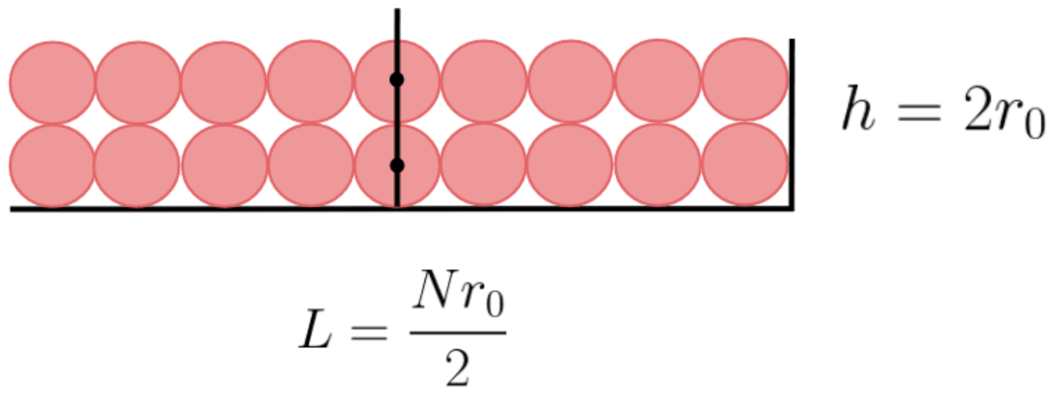

Figure 1 Configuration of the system in the limit of rod.

Another way to calculate the ratio between the radius of gyration of a rod and a circumference it is to approach the two chains from Fig. 1 as a rectangle of width L and height h. The moment of inertia with respect to center of mass is

$$\begin{aligned} I_z &= \int_{-\frac{h}{2}}^{\frac{h}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} (x^2 + y^2)\sigma dx dy, \\ I_z &= \frac{\sigma}{12}(h^3 L + L^3 h). \end{aligned} \tag{53}$$

The superficial density $\sigma = \frac{M}{hL}$, $h = 2r_0$ and $L = Nr_0/2$, we got

$$I_z = \frac{Mr_0^2}{48}(N^2 + 16). \tag{54}$$

The relationship between radius of gyrations and moment of inertia is

$$I_z = MR_g^2, \tag{55}$$

thus

$$R_{g,rod}^2 = \frac{r_0^2}{48}(N^2 + 16). \tag{56}$$

From Eq. (56) we have the ratio

$$\frac{R_{g,rod}}{R_{g,cir}} = \sqrt{\frac{4\pi^2}{48}\left(1 + \frac{16}{N^2}\right)}. \tag{57}$$

For $N \gg 1$

$$\frac{R_{g,rod}}{R_{g,cir}} = \frac{\pi}{2\sqrt{3}} = 0.90689. \tag{58}$$

5 Movie Captions

- Movie 1: Active ring in RUN state. Time is in units of τ_0. Frames are separated by $0.3\tau_0$. Set parameters: $N = 20$, $B = 0$, $Fn = 1$. → Fig 3a
- Movie 2: Active ring in ROT state. Time is in units of τ_0. Frames are separated by $0.3\tau_0$. Set parameters: $N = 20$, $B = 0$, $Fn = 1$. → Fig 3b
- Movie 3: Active ring in PRW state. Time is in units of τ_0. Frames are separated by $0.3\tau_0$. Set parameters: $N = 20$, $B = 0$, $Fn = 1$. → Fig 3c
- Movie 4: Active ring in RRM state. Time is in units of τ_0. Frames are separated by $0.3\tau_0$. Set parameters: $N = 20$, $B = 0$, $Fn = 1$. → Fig 3d
- Movie 5: Active ring in RUN state. Time is in units of τ_0. Frames are separated by $0.3\tau_0$. Set parameters: $N = 100$, $B = 0$, $Fn = 100$, $Pe = 5$, $\tau = 0.1$. → Fig 12

References

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