Stationary States of an Active Brownian Particle
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In this report, we are looking at the stationary state solutions of Active Brownian Particles in a Harmonic Trap [1]. Active Brownian Particle (ABP) is a model for self-propelled motion in a dissipative environment. In an ABP model, particle self-propels in a particular direction $\hat{\boldsymbol{u}}$ with constant speed u_0. The unit vector $\hat{\boldsymbol{u}}$ gets reoriented due to thermal noise which is uncorrelated and Gaussian.

We are considering an ABP in a harmonic trap with potential energy given as :

$$U(\boldsymbol{r}) = \frac{\kappa}{2} r^2 \tag{1}$$

We have the active, instantaneous propulsion vector as :

$$\boldsymbol{u} = u_0 \hat{\boldsymbol{u}} \tag{2}$$

The translational and rotational diffusivities of the particle are written as :

$$D_t = \frac{k_B T}{\zeta_t} \quad ; \quad D_r = \frac{k_B T}{\zeta_r} \tag{3}$$

We also have two Gaussian white noise terms which are uncorrelated and have zero mean.

$$\langle \boldsymbol{\eta}_t(t) \boldsymbol{\eta}_t(t') \rangle = \langle \boldsymbol{\eta}_r(t) \boldsymbol{\eta}_r(t') \rangle = \delta(t - t') \tag{4}$$

We can write the Langevin equations of the system are given as :

$$\frac{d\boldsymbol{r}}{dt} = u_0 \hat{\boldsymbol{u}} - k\boldsymbol{r} + \sqrt{2D_t} \boldsymbol{\eta}_t(t) \tag{5}$$

$$\frac{d\hat{\boldsymbol{u}}}{dt} = \sqrt{2D_r} \boldsymbol{\eta}_r(t) \times \hat{\boldsymbol{u}}(t) \tag{6}$$

The corresponding Fokker-Planck equation for the probability distribution function $P(\boldsymbol{r}, \hat{\boldsymbol{u}}, t)$ is given by :

$$\frac{\partial P}{\partial t} = -\nabla \cdot \boldsymbol{J}_t + D_r \nabla^2_{\hat{\boldsymbol{u}}} P \tag{7}$$

where,

$$\boldsymbol{J}_t = \left(-D_t \nabla + \boldsymbol{v}\right) P \quad ; \quad \boldsymbol{v} = u_0 \hat{\boldsymbol{u}} - k\boldsymbol{r} \tag{8}$$

In the stationary state, the LHS of equation (7) goes to zero.

$$\therefore \nabla \cdot \boldsymbol{J}_t = D_r \nabla^2_{\hat{\boldsymbol{u}}} P \tag{9}$$

Now, we want to obtain a solution of the Fokker-Planck equation. To do that, first we define the marginal probability density of the particle's position.

$$\Phi(\boldsymbol{r}) = \int P(\boldsymbol{r}, \hat{\boldsymbol{u}}) d^d \hat{\boldsymbol{u}} \tag{10}$$

It satisfies the equation :

$$\nabla \cdot \boldsymbol{K} = 0 \quad ; \quad \boldsymbol{K}(\boldsymbol{r}) = -D_t \nabla \Phi + \left(u_0 \overline{\hat{\boldsymbol{u}}} - k\boldsymbol{r}\right) \Phi(\boldsymbol{r}) \tag{11}$$

where,

$$\overline{\hat{\boldsymbol{u}}} = \Phi(\boldsymbol{r})^{-1} \int \hat{\boldsymbol{u}} P(\boldsymbol{r}, \hat{\boldsymbol{u}}) d^d \hat{\boldsymbol{u}} \tag{12}$$

Using the radial symmetry of the system, we arrive at the following conclusions :

$$\boldsymbol{K}(\boldsymbol{r}) = 0 \quad : \quad \text{identically} \tag{13}$$

$$\overline{\hat{\boldsymbol{u}}}(\boldsymbol{r}) = g(r) \hat{\boldsymbol{r}} \quad ; \quad g(r) \leq 1 \tag{14}$$

Keeping these conditions in mind, we can set the $\boldsymbol{K} = 0$ in equation (11) and obtain the solution.

$$\Phi(r) = \Phi(0) \exp\left(\frac{u_0}{D_t} \int_0^r g(r') dr' - \frac{\kappa r^2}{2k_B T}\right) \tag{15}$$

This is essentially the equilibrium Boltzmann distribution modified by activity.

We can also solve equation (11) in terms of dimensionless quantities.

$$\boldsymbol{r}' = \frac{\boldsymbol{r}}{r_m} \quad ; \quad r_m = \frac{u_0}{k} \tag{16}$$

$$D_t' = \frac{D_t k}{u_0^2} \quad ; \nabla' = r_m \nabla \tag{17}$$

Writing equation (11) in terms of the dimensionless quantities :

$$-D_t' \nabla' \Phi(r') + \left(g(r') - r'\right) \Phi(r') = 0 \tag{18}$$

We can solve the equation in two regimes, based on the value of D_t' : the strongly active regime ($D_t' \longrightarrow 0$) and the regime of non-zero translational diffusion ($D_t' > 0$).

In the strongly active limit, the gradient term in equation (18) can be neglected when compared to the second term. So, we obtain a relation :

$$g(r) = \frac{r}{r_m} \quad \Longrightarrow \quad \overline{\hat{\boldsymbol{u}}} \backsimeq \frac{\boldsymbol{r}}{r_m} \tag{19}$$

Now, to solve for $\Phi(r)$, we can multiply equation (9), the stationary state equation with $\boldsymbol{v}$ in equation (8) and the integrate over $\hat{\boldsymbol{u}}$.

We obtain the final general solution as :

$$u_0^2 \int \hat{\boldsymbol{u}} \left(\hat{\boldsymbol{u}} \cdot \nabla P\right) d^d \hat{\boldsymbol{u}} + k\alpha \boldsymbol{r} \Phi(\boldsymbol{r}) - k^2 \boldsymbol{r} \left(\boldsymbol{r} \cdot \nabla \Phi\right) = 0 \tag{20}$$

where,

$$\alpha = D_r (d - 1) - (d + 1) k \tag{21}$$

To get some exact solutions to the Fokker-Planck equations, we will now focus on ABP in two dimensions with Gaussian approximations.

There are three degrees of freedom for the particle in this case. Two plane polar coordinates (r, ϕ) characterize the position vector and the orientation angle θ characterizes the unit propulsion vector $\hat{\boldsymbol{u}} = (\cos\theta, \sin\theta)$.

Dynamics of θ are then given as :

$$\frac{d\theta}{dt} = \sqrt{2D_r}\eta_\theta(t) \tag{22}$$

Using the radial symmetry, we can write $P(r, \theta, \phi) = P(r, \chi)$, where $\chi = \theta - \phi$. We can also separate the variables as :

$$P(r, \chi) = \Phi(r) f(\chi|r) \tag{23}$$

Using radial components, we can write the exact Fokker-Planck equation for the strongly active limit as :

$$\sigma^2_{\cos\chi}\Phi'(r) + \left[\partial_r \sigma^2_{\cos\chi} + \frac{2\sigma^2_{\cos\chi}}{r} - \frac{1}{r} + \left(\frac{\alpha}{k} + 4\right)\frac{r}{r_m^2}\right]\Phi(r) = 0 \tag{24}$$

Making a Gaussian estimate for χ :

$$\sigma^2_{\cos\chi} \backsimeq \frac{1}{2}\left(1 - \frac{r^2}{r_m^2}\right)^2 \tag{25}$$

This assumption gives us the solution for $r < r_m$ as :

$$\Phi(r) \backsimeq C\left[1 - \frac{r^2}{r_m^2}\right]^{-3} \exp\left[-\frac{1}{\beta}\left(1 - \frac{r^2}{r_m^2}\right)^{-1}\right] \quad ; \quad \beta = \frac{k}{D_r} \tag{26}$$

C is a constant which is fixed by the normalisation condition :

$$\int_0^{r_m} \Phi(r) 2\pi r dr = 1 \tag{27}$$

It is calculated to be :

$$C = \frac{1}{\pi r_m^2 \beta^2}\left(\frac{1}{\beta} + 1\right)^{-1} \exp\left(\frac{1}{\beta}\right) \tag{28}$$

On plotting equation (26), we observe that there is a transition between the concave and convex probability distribution.

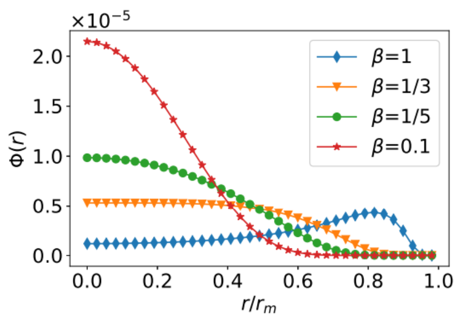

Fig 1. Plot of $\Phi(r)$ for four different values of β. [1]

To better understand the transition between the concave and the convex shaped distributions, the zeroes of the first derivatuve of $\Phi(r)$ were calculated.

$$r = 0 \quad ; \quad r = r_m\sqrt{1 - \frac{1}{3\beta}} \tag{29}$$

So, we can conclude the peak of the distributions to be given as :

$$r_{max} = 0 \quad : \quad \beta \leq \frac{1}{3} \tag{30}$$

$$r_{max} = r_m\sqrt{1 - \frac{1}{3\beta}} \quad : \quad \beta > \frac{1}{3} \tag{31}$$

Thus, the probability distribution undergoes a phase transition-like change between concave and convex shapes as β increases beyond the critical value of $\beta_c = \frac{1}{3}$. We need to note that both of these distributions are non-Gaussian in the strong activity region $D_t' \longrightarrow 0$. As D_t' is increased, both cross over to the asymptotic Gaussian form.

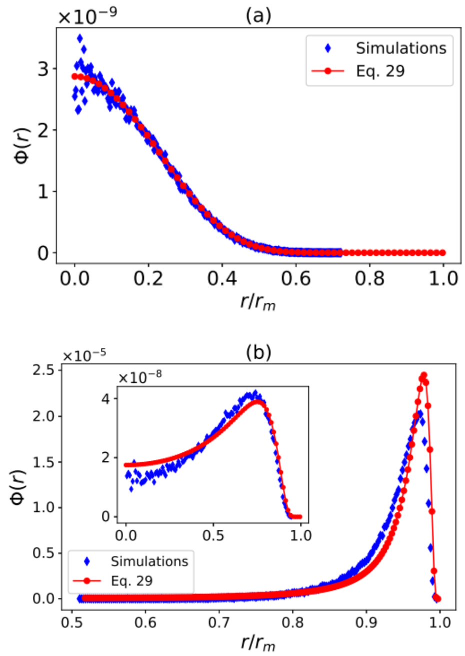

Fig 2. Simulation plots for different β values. [1]

Some numerical simulations were carried out, for different values of trap stiffness, which replicated the analytic results.

In conclusion, we can have a schematic phase diagram for the system as follows :

(a) Active Concave : $\Phi(r)$ is maximum at trap centre but is non-Gaussian in general.

(b) Active Convex : $\Phi(r)$ has maximum away from trap centre, and has either a minima or local subdominant maxima at that position.

(c) Passive, non-equilibrium phase : $\Phi(r)$ is Gaussian and resembles the equilibrium Boltzmann form.

References

[1] Stationary States of an Active Brownian particle in a harmonic trap; Urvashi Nakul, Manoj Gopalakrishnan https://arxiv.org/abs/2209.09184