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On the mean square displacement of an active Brownian particle with rotational inertia in a harmonic trap

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One of the unsolved problems in the physics of active matter is providing an analytical description of the mean square displacement of an active Brownian particle in a harmonic trap that takes into account the particle's translational and rotational inertia. Solving this problem is relevant because inertial effects can play a significant role in a number of experiments and applications involving active particles. Within the framework of an active Brownian particle model with translational and rotational inertia, an analytical expression describing the evolution of the mean square displacement of a particle in a harmonic trap has been obtained.

Keywords: active matter; active Brownian particles; mean square displacement.

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Introduction

Active matter is a special form of “soft” condensed matter, which represents a dispersion medium containing finely dispersed active particles. Despite their simplicity and lack of moving parts, such particles (also called nano- and micromotors) can autonomously convert environmental energy into directed motion [1–3]. Systems of such particles are of great interest for statistical mechanics and materials science and have numerous promising applications, from purely technical to biomedical ones. Synthetic active particles are ideal building blocks for the dynamic self-assembly of new-generation functional microstructures capable of performing specific tasks autonomously and in a targeted manner. Colloidal active matter is promising in the context of developing new materials with a “programmable” response. Applications related to biochemical analysis, substance separation, collective cargo delivery, and energy utilization from chaotic motion are also being developed [1, 2].

One of the unresolved fundamental problems in active matter physics is the analytical

description of the mean square displacement, $\text{MSD}(t)$, of an active Brownian particle in a harmonic potential, taking into account both the translational and rotational inertia of the particle. Solving this problem is of high relevance due to numerous experiments with active particles where inertial effects can play a significant role [4–9]. At present, the problem has been solved only for a number of specific (limiting) cases, namely: $\text{MSD}(t)$ of an inertia-free active Brownian particle in a trap [10–15]; $\text{MSD}(t)$ of an active Ornstein-Uhlenbeck particle with translational inertia in a trap [16, 17]; $\text{MSD}(t)$ of a free, fully inertial active Brownian particle (with both translational and rotational inertia) [18, 19]; and $\text{MSD}(\text{at } t = \infty)$ of a fully inertial active Brownian particle in a trap [20].

This paper is the first to derive an exact analytical expression describing the evolution of the mean square displacement, $\text{MSD}(t)$, of a fully inertial active Brownian particle in a harmonic trap.

Basic Equations

Within the model of an active Brownian

particle with translational and rotational inertia, the two-dimensional motion of a spherical particle (with mass M and moment of inertia J) in a harmonic trap (characterized by frequency ω_0) projected onto an arbitrary X -axis is described by the following equations [18–20]:

$$M\ddot{x}(t) = -\nu_t M\dot{x}(t) + F_A \cos(\phi(t)) - M\omega_0^2 x(t) + F_B^{(x)}, \quad (1)$$

$$\ddot{\phi}(t) = -\nu_r (\dot{\phi}(t) + \sqrt{2D_r} \zeta_r(t)), \quad (2)$$

where ν_t and ν_r are damping coefficients for the translational and rotational motion of the particle in a viscous medium; F_A is active (propulsive) force, whose direction is determined by orientational angle $\phi(t)$ measured from X axis; $F_B^{(x)}$ is x component of the Brownian force (“translational” noise); $D_r = T / (\nu_r J)$ is rotational diffusion coefficient (here, T is the medium temperature expressed in energy units); and ζ_r is Gaussian white noise with zero mean and unit variance.

In the stationary state, the time-dependent mean square displacement of the particle along X axis is defined as

$$\text{MSD}(t) \equiv \langle [x(t) - x(0)]^2 \rangle = 2\langle x^2 \rangle - 2\langle x(t)x(0) \rangle, \quad (3)$$

where $\langle x(t)x(0) \rangle$ is auto-correlation function of the particle position. Note that $\text{MSD}(\infty) = 2\langle x^2 \rangle$. Since the “translational” and “rotational” noises do not correlate, $\text{MSD}(t)$ can be written as the sum of two terms: the first term is the well-known Uhlenbeck–Ornstein formula for a passive Brownian particle [21], and the second term is the result of the contribution from the active (propulsive) force. Here, we intentionally disable the translational noise (setting $F_B = 0$) to focus on studying the contribution of the active force.

According to the Khinchin–Kolmogorov theorem, the autocorrelation function of the particle position can be written as

$$\langle x(t)x(0) \rangle = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-i\omega t} H^2(\omega) S(\omega) d\omega, \quad (4)$$

where $H(\omega) = (F_A / M) / (\omega_0^2 - \omega^2 + i\nu_t \omega)$ is transfer function, and $S(\omega)$ is power spectral density of the process $\cos(\phi(t))$. For a stationary process, the power spectral density is written as the Fourier transform of the autocorrelation function:

$$S(\omega) = 2 \int_0^\infty \cos(\omega t) \langle \cos(\phi(t)) \cos(\phi(0)) \rangle dt, \quad (5)$$

where the autocorrelation function looks as follows [19, 20]

$$\begin{aligned} \langle \cos(\phi(t)) \cos(\phi(0)) \rangle &= \\ &= \frac{1}{2} \exp \left[-\frac{D_r}{\nu_r} (\nu_r t - 1 + e^{-\nu_r t}) \right]. \end{aligned} \quad (6)$$

Results and Discussion

Integrating equation (5) after expanding the autocorrelation function (6) into a series allows deriving the power spectral density of the process $\cos(\phi(t))$ in the stationary state:

$$S(\omega) = e^{D_r/\nu_r} \sum_{m=0}^{\infty} \frac{(-D_r/\nu_r)^m}{m!} \frac{D_r + m\nu_r}{(D_r + m\nu_r)^2 + \omega^2}. \quad (7)$$

Substituting transfer function $H(\omega)$ and expression (7) into equation (4), and applying the residue theorem, we obtained the following formulas.

For non-oscillatory particle motion in the trap ($\omega_0 / \nu_t < 1/2$),

$$\begin{aligned} \langle x(t)x(0) \rangle &= \frac{V_0^2 \alpha e^\xi}{8\omega_0^2} \times \\ &\times \left\{ e^{-\frac{\nu_t t}{2}} \left[C_+ G_1 e^{\tilde{\Omega} t} + C_- G_2 e^{-\tilde{\Omega} t} \right] + \right. \\ &\left. + e^{-D_r t} \left[C_+ F_1(t) + C_- F_2(t) \right] \right\}, \end{aligned} \quad (8a)$$

where $V_0 = F_A / M\nu_t$ is the self-propulsion velocity of the particle, which is calculated from the formal balance of active and dissipative forces in the absence of translational and rotational noises; $\alpha = \nu_t / \nu_r$, $\xi = D_r / \nu_r$, $C_+ = 1 + 0.5\nu_t / \tilde{\Omega}$,

$C_- = 1 - 0,5v_t / \tilde{\Omega}$, $\tilde{\Omega} = \sqrt{v^2 / 4 - \omega_0^2}$,
 $G_j = \xi^{-a_j} \gamma(a_j, \xi) + \xi^{-b_j} \gamma(b_j, \xi)$ and $F_j(t) =$
 $= z^{-a_j}(t) \gamma(a_j, z(t)) - z^{-b_j}(t) \gamma(b_j, z(t))$, here
 $a_j = \xi + i\omega_j / v_r$, $b_j = \xi - i\omega_j / v_r$, $z(t) = \xi e^{-v_r t}$,
 $\omega_{1,2} = -iv_t / 2 \pm i\tilde{\Omega}$, a $\gamma(s, z) = \int_0^z y^{s-1} e^{-y} dy$ is the
lower incomplete gamma function.

In the oscillatory motion regime ($\omega_0 / v_t > 1/2$),

$$\begin{aligned}
 \langle x(t)x(0) \rangle &= \frac{V_0^2 \alpha e^\xi}{4\omega_0^2} \times \\
 &\times \left\{ e^{-\frac{v_t t}{2}} \left[\left(\text{Re}[G_2] + \frac{v_t}{2\Omega} \text{Im}[G_2] \right) \cos(\Omega t) + \right. \right. \\
 &\quad \left. \left. + \left(\frac{v_t}{2\Omega} \text{Re}[G_2] - \text{Im}[G_2] \right) \sin(\Omega t) \right] + \right. \\
 &\quad \left. + e^{-D_r t} \left(\text{Re}[F_2(t)] + \frac{v_t}{2\Omega} \text{Im}[F_2(t)] \right) \right\}, \quad (8b)
 \end{aligned}$$

where $\text{Re}[\dots]$ and $\text{Im}[\dots]$ are real and imaginary parts of complex functions, and $\Omega = i\tilde{\Omega}$.

In the stationary state at $t=0$, function $\langle x(t)x(0) \rangle$ describes the mean square position of the particle relative to the trap center:

$$\langle x^2 \rangle = \frac{V_0^2 \alpha e^\xi}{4\omega_0^2} \left\{ C_+ \frac{\gamma(a_1, \xi)}{\xi^{a_1}} + C_- \frac{\gamma(a_2, \xi)}{\xi^{a_2}} \right\} \quad \text{for} \quad \omega_0 / v_t < 1/2, \quad (9a)$$

and

$$\langle x^2 \rangle = \frac{V_0^2 \alpha e^\xi}{2\omega_0^2} \left\{ \text{Re} \left[\frac{\gamma(a_2, \xi)}{\xi^{a_2}} \right] + \frac{v_t}{2\Omega} \text{Im} \left[\frac{\gamma(a_2, \xi)}{\xi^{a_2}} \right] \right\} \quad \text{for } \omega_0 / v_t > 1/2. \quad (9b)$$

Now, to calculate the evolution function of the particle's mean square displacement in the stationary state, $\text{MSD}(t)$, it is sufficient to substitute (8)–(9) into (3).

It is important to note that equations (9a) and (9b) coincide with those previously obtained in paper [20] and verified against the numerical simulation results. It can also be easily shown that when $v_r \rightarrow \infty$, equation (8a) reduces to the

known autocorrelation function $\langle x(t)x(0) \rangle_{\text{AOUP}}$ for the active Ornstein-Uhlenbeck particle model, which is often used for the approximate description of active Brownian particle dynamics with only translational inertia considered [16, 17]. When $\omega_0 = 0$, the expression for $\text{MSD}(t)$ can be reduced to the formula derived in paper [19] for a free, fully inertial active Brownian particle. The listed facts confirm that the formulas derived in this paper are correct.

With high trap frequency ($\omega_0 \rightarrow \infty$) at times $t \gg \omega_0^{-1}$, the expression applying to particle's $\text{MSD}(t)$ and described by formulas (3), (8b), and (9b), becomes significantly simpler and can be represented in terms of elementary functions:

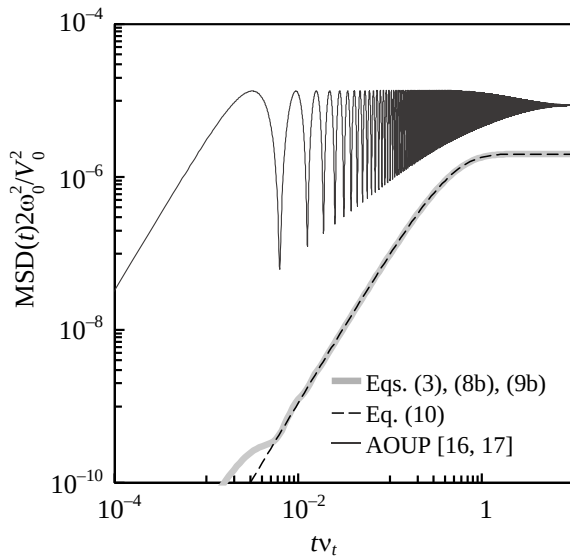
$$\begin{aligned}
 \text{MSD}(t) &\approx \text{MSD}(\infty) \times \\
 &\times \left\{ 1 - \exp \left[-\frac{D_r}{v_r} (v_r t - 1 + e^{-v_r t}) \right] \right\}, \quad (10)
 \end{aligned}$$

where

$$\text{MSD}(\infty) = \frac{(V_0 v_t)^2}{\omega_0^4}. \quad (11)$$

An interesting feature is the absence of oscillations in formula (10), which are specific to the mean square displacement evolution for both passive particles [21] and active Ornstein-Uhlenbeck particles [16]. The figure shows normalized $\text{MSD}(t)$ for a spherical active Brownian particle with $D_r / v_r = 1$ and $\omega_0 / v_t = 1000$. For comparison, $\text{MSD}(t)$ for the active Ornstein-Uhlenbeck particle (AOUP) with $\omega_0 / v_t = 1000$ and without considering the particle's rotational inertia is added to the figure.

It is easy to see that within a strong trap, $\text{MSD}(\infty)$ of a fully inertial active particle does not depend on v_r , and therefore, on particle's rotational inertia. Furthermore, $\text{MSD}(\infty)$ coincides with the mean square displacement of the active Ornstein-Uhlenbeck particle [16] when $tv_t \gg 1$ and $D_r / v_t \ll 1$. The latter is true, for example, for a particle with a radius of $\sim 1 \mu\text{m}$ in a gas at a pressure of $\sim 1000 \text{ Pa}$ or higher.



Normalized mean square displacement of an active particle at $\omega_0/\nu_t = 1000$ as a function of time. The thick solid line represents the fully inertial model with $D_r/\nu_t = 1$; the thin solid line represents the AOUP model without accounting for the particle's rotational inertia.

Conclusion

Analytical expressions describing the evolution of a particle's mean square displacement in a harmonic trap have been derived for the first time within the framework of

the active Brownian particle model with translational and rotational inertia. The results of this paper can be useful for describing the dynamics of light-sensitive active microparticles in gas discharge plasmas [4, 5], superfluid helium [6], and vacuum optical traps [22], as well as microswimmers in acoustic traps [23], macroscopic vibrobots in parabolic confinement [9], and others. Macroscopic inertial active particles driven by vibration and moving along finite trajectories can be used as a controllable analogue of vehicles or pedestrians for modeling congestion at bottlenecks in optimizing transportation systems and designing public spaces [24]. Macroscopic inertial active particles can be used in creating mechanical metamaterials and autonomous devices driven by vibration [25, 26]. Ideas for creating microscopic heat engines based on inertial active matter are also discussed [27, 28].

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