Swarming in three dimensions

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We consider a three-dimensional model of active Brownian particles interacting via a Morse-type potential. The system exhibits two modes of motion: translation and a coherent rotation in a torus-shape structure. We observe noise-induced transitions in both directions between the two states. These occur at different noise intensities, thus leading to a hysteresis curve. For certain parameter regions, the system switches persistently between the states such that the center of mass alternates between ballistic and diffusive motion. The coherent rotation leads to a pronounced mean angular momentum that changes its direction diffusively. We derive an analytic expression for the diffusion of the angular momentum of one particle in an external harmonic potential and show that it is always faster than the stochastic switching of the direction of motion in the two-dimensional case.

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I. INTRODUCTION

Various species of animals assemble in flocks or herds that self-organize without a leader [1,2]. Birds and fish [3] are common examples, but also insects [4], locusts [5], daphnia [6], and bacteria [7] show this kind of behavior.

There are two main approaches commonly used to describe collective motion: a continuum and an individual-based one. Continuum models typically describe swarms by a density function $\rho(\vec{r})$ and a velocity vector field $\vec{u}(\vec{r})$ [8–12]. Individual or agent-based models use differential equations [13–15] or discrete time evolution algorithms [16] for each particle and consider ensembles of interacting objects.

Both types of models exhibit various types of collective motion, which can be classified as a mobile state with a nonzero center-of-mass velocity and an immobile state with a fixed center of mass. In the immobile state, we can further distinguish between disordered and collective, for example rotational, motion of the individual particles. Depending on the parameters of these models such as density or noise, phase transitions between the different states are observed.

One common transition, on which we will focus in the present work, is a noise-induced transition from translation to rotation [17]. However, there are few studies concerning the backwards transition from rotation to translation, since in most cases the mobile state rather than the immobile state proves unstable [18,19]. Kolpas *et al.* [20] found this transition in one spatial dimension with discrete zones of interaction. Huepe *et al.* [21] studied a two-dimensional system with velocity alignment and found bursts of disordered motion in the ordered phase.

In the present paper, we extend a particle-oriented algorithm to three spatial dimensions. Compared to the two-dimensional case, we elaborate on two findings.

First we consider a set of N identical self-propelled particles interacting globally via a pair potential. We find that adding a repulsive part to the interaction leads to noise-induced transitions not only from translation to rotation but also vice versa. These transitions occur at different noise intensities, thus leading to a hysteresis curve. This effect was not observed so far in two dimensions, where the rotation was stable even without noise. The aim of our study is to investigate the dependence of the critical noise intensity on the system parameters. For a certain parameter region, the critical noise intensities almost coincide. Then the system switches spontaneously between the two states.

In two dimensions, the rotational motion of the particles is restricted to clockwise or counterclockwise direction. To perform a stochastic switch between the two directions, the particle has to cross a barrier where the angular momentum goes through zero. A new effect that occurs in the three-dimensional case is the diffusion of the angular momentum. The particle can change its direction of motion continuously. We analyze the diffusion of the angular momentum of one particle in a three-dimensional external harmonic potential and compare our results to the two-dimensional case. We will show that the diffusion of the angular momentum in three dimensions leads to a faster change of the rotational direction than the switching in two dimensions, regardless of the noise intensity.

II. MODEL

We consider a set of N identical active Brownian particles [22,23] in three-dimensional space with positions $\vec{r}_i$, velocities $\vec{v}_i$ $(i=1,\ldots,N)$, and unit mass. The equations of motion read

$$\dot{\vec{r}}_i = \vec{v}_i, \tag{1a}$$

$$\dot{\vec{v}}_i = -\gamma(\vec{v}_i)\vec{v}_i - \sum_{\substack{k=1\\k\neq i}}^{N} \vec{\nabla}_i U_{\mathrm{M}}(\vec{r}_i - \vec{r}_k) + \sqrt{2D}\vec{\xi}_i. \tag{1b}$$

The particles are subject to a friction force $\gamma(\vec{v})$, which consists of a positive and a negative part. The negative part serves as an energy pump, thus accounting for the active motion of the agents. We use the Rayleigh friction [24]

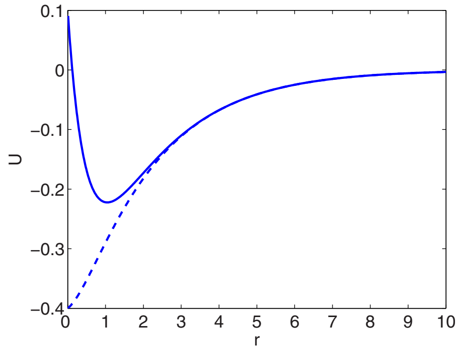

FIG. 1. (Color online) Morse potential as a function of the absolute value of the distance of two particles for two different sets of parameters: $C_r=0.6$ (solid line), $C_r=0.1$ (dashed line). Other parameter values: $l_r=0.5$, $l_a=2.0$, $C_a=0.5$.

$$\gamma(\vec{v}) = -\gamma_1 + \gamma_2(\vec{v}\cdot\vec{v}), \tag{2}$$

which in the absence of other forces results in a stationary velocity $v_0=\sqrt{\frac{\gamma_1}{\gamma_2}}$. A biological motivation for this type of friction is given in [25,26].

The last term in Eq. (1b) is a stochastic force of intensity D which models the individual behavior of the agents. The forces $\vec{\xi}_i$ are independent for different particles and characterized by the correlation functions

$$\langle \xi_{n,i}(t)\rangle = 0, \quad \langle \xi_{n,i}(t)\xi_{m,j}(t')\rangle = \delta_{ij}\delta_{nm}\delta(t-t'), \tag{3}$$

with $i,j \in 1,\ldots,N$; $n,m \in x,y,z$.

We use two types of potentials. In the first part of this work, the particles interact globally via a pair potential. A generalized Morse potential [27] captures fundamental properties of swarming animals. At short range, the potential has to be repulsive to avoid collisions and to prevent the agents from interpenetrating each other. An attractive force mimics the aim of the individual to stay with the group. The attraction should be of long range, but eventually approach zero to account for the limited sensing range of animals. An exponentially decaying function meets both demands. Therefore, we introduce a generalized Morse potential (see Fig. 1), which consists of an attractive and a repulsive part. Both are exponential functions with amplitudes C_a and C_r and ranges l_a and l_r, respectively,

$$U_{\mathrm{M}}(\vec{r}_i-\vec{r}_k) = C_r e^{-|\vec{r}_i-\vec{r}_k|/l_r} - C_a e^{-|\vec{r}_i-\vec{r}_k|/l_a}. \tag{4}$$

The equilibrium distance of two particles is

$$r_0 = \frac{l_r l_a}{l_r - l_a}\ln\left(\frac{l_r C_a}{l_a C_r}\right). \tag{5}$$

For $\frac{l_r}{l_a}<1$, the potential possesses a minimum corresponding to short-range repulsion and long-range attraction. One can see that for $\frac{l_r}{l_a}<1$ and $\frac{l_r}{l_a}>\frac{C_r}{C_a}$, the minimum would shift to negative values. Since the absolute value of the interparticle distance in Eq. (4) is positive, the potential is attractive everywhere. Therefore, we will concentrate on the parameter space where $\frac{l_r}{l_a}<1$ and $\frac{l_r}{l_a}<\frac{C_r}{C_a}$.

For the consideration of the diffusion of the angular momentum in three dimensions, we investigate one particle in an external harmonic potential. For this model, the equations of motion read

$$\dot{\vec{r}} = \vec{v}, \tag{6a}$$

$$\dot{\vec{v}} = -\gamma(\vec{v})\vec{v} - \omega^2\vec{r} + \sqrt{2D}\vec{\xi}. \tag{6b}$$

In the two-dimensional case, the particle can rotate only clockwise or counterclockwise. Its angular momentum cannot change its direction continuously, but has to perform a stochastic switch. In three dimensions, the particle rotates on the surface of a sphere such that the absolute value of its angular momentum is almost fixed, but its direction diffuses.

III. NOISE-INDUCED SWITCHINGS BETWEEN TRANSLATIONAL AND ROTATIONAL MOTION

A. Hysteresis

Depending on the parameters, the system displays two different modes of motion: a translational mode and a rotational mode. To study the transition from translation to rotation, we prepare the system in the translational mode in an arbitrary direction. In this mode, the particles move parallel with their stationary velocity $v_0=\sqrt{\frac{\gamma_1}{\gamma_2}}$. The spatial configuration in the center-of-mass system corresponds to the equilibrium configuration. Without noise, there are no fluctuations; the center of mass moves with v_0. Increasing the noise gives rise to fluctuations and leads to a decreasing velocity of the center of mass [28]. Above a critical noise value $D_{\mathrm{crit}}^{\mathrm{trans}}$ the translational motion breaks down and the particles start to rotate around the center of mass. Whereas for a harmonic potential the particles rotate in any direction on the equipotential sphere, the interaction leads to coherent motion in a torus shape structure, with the orientation depending on the initial conditions (Fig. 2). The center of mass moves diffusively, therefore the absolute value of its velocity is not zero and increases with the noise intensity. Starting from the rotational state and decreasing the noise intensity, the system exhibits a transition to the translational mode at a different critical noise value $D_{\mathrm{crit}}^{\mathrm{rot}}$. Surprisingly, this second transition back to translation was not observed in the two-dimensional case. In general, the transitions occur at different noise values, which leads to a hysteresis curve (Fig. 3). The decrease of the center-of-mass velocity with rising noise intensity can be shown by considering the equation of motion of the center-of-mass velocity $\vec{u}=\frac{1}{N}\sum_{i=1}^{N}\vec{v}_i$, whose absolute value will be labeled as $u=|\vec{u}|$. Analogously, the absolute value of the velocity of the ith particle will be labeled as $v_i=|\vec{v}_i|$. The ensemble average of Eq. (1b) yields

$$\dot{\vec{u}} = \gamma_1\vec{u} - \gamma_2\frac{1}{N}\sum_{i=1}^{N} v_i^2\vec{v}_i. \tag{7}$$

The interaction potential is pairwise and therefore averages to zero. The noise intensity decreases when increasing the number of particles and is negligible compared to the

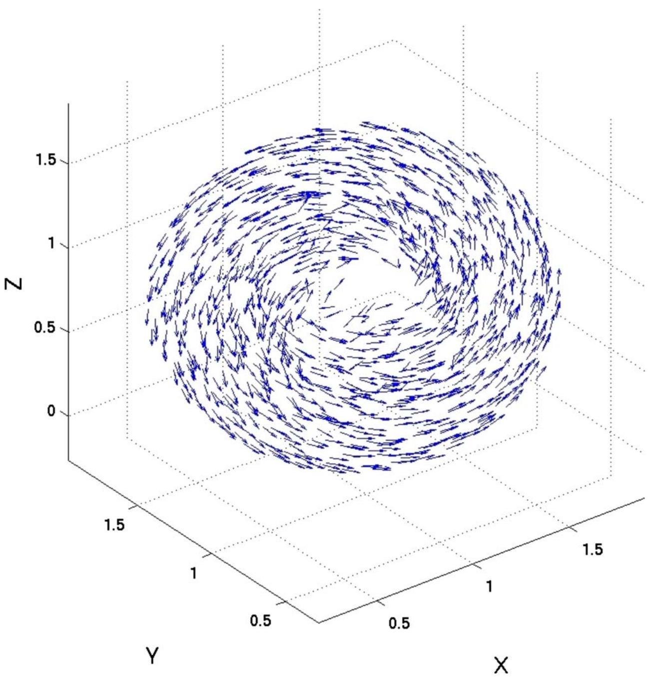

FIG. 2. (Color online) Rotational mode: particles move coherently in a torus shape structure. Parameter values: $N=1000$, $\gamma_1=1.6$, $\gamma_2=0.5$, $C_r=C_a=l_r=0.5$, $l_a=2.0$, $D=0$.

fluctuations of the individual particles. The velocity of each particle can be written as the mean velocity plus some deviation $\delta\vec{v}_i$, which average to zero. According to [28], the average of the third moment of the velocity deviations $\langle \delta v_i^2 \delta\vec{v}_i \rangle$ in two spatial dimensions is small compared to the other terms and can therefore be neglected. This has also been confirmed by numerical simulations for three spatial dimensions. From this follows

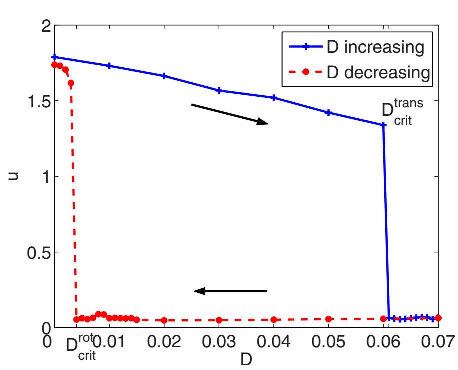

FIG. 3. (Color online) Hysteresis curve of the absolute value of the center-of-mass velocity u versus noise intensity D. The solid (blue) line represents increasing noise intensity, the dashed (red) line represents decreasing noise intensity. Note the increase of the center-of-mass velocity with the noise intensity due to its diffusive motion in the rotational mode ($u \approx 0$) and, respectively its decrease due to fluctuations in the translational mode ($u \gg 0$). Parameter values: $N=100, \gamma_1=1.6, \gamma_2=0.5, C_r=C_a=l_r=0.5, l_a=2.0$.

$$\begin{aligned}\frac{1}{N}\sum_{i=1}^{N} v_i^2\vec{v}_i &= \frac{1}{N}\sum_{i=1}^{N}[(\vec{u}+\delta\vec{v}_i)\cdot(\vec{u}+\delta\vec{v}_i)](\vec{u}+\delta\vec{v}_i)\\ &= u^2\vec{u} + \frac{1}{N}\sum_{i=1}^{N}\vec{u}\,\delta v_i^2\\ &\quad + \frac{1}{N}\sum_{i=1}^{N}2(\vec{u}\cdot\delta\vec{v}_i)\delta\vec{v}_i + \frac{1}{N}\sum_{i=1}^{N}\delta v_i^2\delta\vec{v}_i \approx u^2\vec{u}\\ &\quad + \vec{u}\langle(\delta v_i^2)\rangle + 2\langle(\vec{u}\cdot\delta\vec{v}_i)\delta\vec{v}_i\rangle. \end{aligned} \tag{8}$$

To evaluate these mean values, we introduce the components of the velocity fluctuations parallel and perpendicular to the velocity of the center of mass $\delta\vec{v}_{\parallel,i}$ and $\delta\vec{v}_{\perp,i}$ [17] with the absolute values $\delta v_{\parallel,i}$ and $\delta v_{\perp,i}$, such that $\delta\vec{v}_i = \delta\vec{v}_{\parallel,i} + \delta\vec{v}_{\perp,i}$. This yields for the last term in Eq. (8)

$$\begin{aligned}\langle(\vec{u}\cdot\delta\vec{v}_i)\delta\vec{v}_i\rangle &= \langle(\vec{u}\cdot\delta\vec{v}_{\parallel,i})(\delta\vec{v}_{\parallel,i}+\delta\vec{v}_{\perp,i})\rangle\\ &= \vec{u}\langle\delta v_{\parallel,i}^2\rangle + \langle(\vec{u}\cdot\delta\vec{v}_{\parallel,i})\delta\vec{v}_{\perp,i}\rangle. \end{aligned} \tag{9}$$

The friction term leads to a correlation of the components of the velocity and its fluctuations. However, numerical simulations confirm that in first approximation we can neglect the last term in Eq. (9) compared to the first term. We insert this result and Eq. (8) into Eq. (7) and obtain

$$\dot{\vec{u}} = \gamma_1\vec{u} - \gamma_2[u^2\vec{u} + \vec{u}(3\langle\delta v_{\parallel,i}^2\rangle + \langle\delta v_{\perp,i}^2\rangle)]. \tag{10}$$

We find two stationary solutions for the center-of-mass velocity. The first solution corresponds to the rotational mode where the center of mass is at rest,

$$\vec{u} = 0. \tag{11}$$

The second solution corresponds to the translational mode where the center of mass moves with a nonzero velocity in arbitrary direction whose absolute value is fixed to

$$u^2 = \frac{\gamma_1}{\gamma_2} - 3\langle\delta v_\parallel^2\rangle - \langle\delta v_\perp^2\rangle. \tag{12}$$

In the absence of noise, the center of mass moves with the stationary velocity of the particles $v_0 = \sqrt{\frac{\gamma_1}{\gamma_2}}$. Increasing the noise leads to higher velocity deviations, which decreases the center-of-mass velocity. Also the direction of motion of the center of mass is not specified and changes in time due to the noise.

The discontinuity of the center-of-mass velocity allows us to clearly distinguish the two states. Since it is also easy to measure, we use it as an order parameter for the system.

B. Influence of a repulsive potential

For the transition from rotation to translation, the critical noise value decreases with increasing $\frac{C_r}{C_a}$. However, for $\frac{l_r}{l_a} < \frac{C_r}{C_a} < 1$ the critical noise value decreases with decreasing $\frac{C_r}{C_a}$; below $\frac{C_r}{C_a} = \frac{l_r}{l_a}$, no transition to translation takes place. In this parameter range, the potential does not possess a

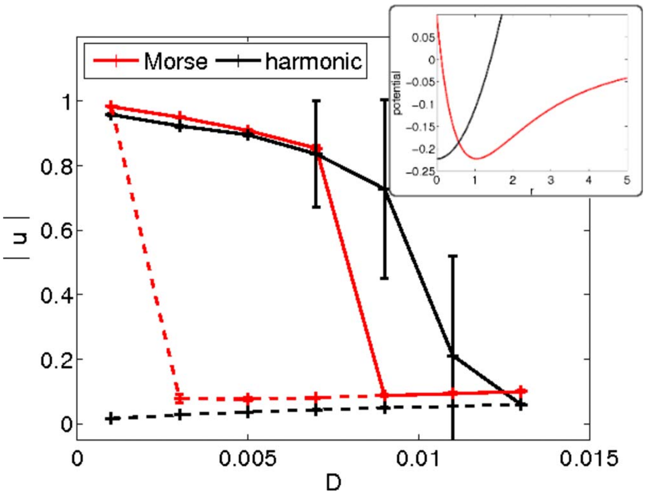

FIG. 4. (Color online) Absolute value of the mean center-of-mass velocity versus noise intensity for a Morse potential [gray (red)] and a harmonic potential (black). Solid lines represent increasing noise intensities, dashed lines represent decreasing noise intensities. In the case of the harmonic potential, the system shows only the transition from translation to rotation [28]. The latter is stable even without noise. Including an equilibrium distance (i.e., a repulsive part) leads to an additional transition from rotation back to translation. Parameter values: $N=20, \gamma_1=\gamma_2=1$; Morse: $C_r=0.6, C_a=l_r=0.5, l_a=2.0$; harmonic: $a=0.1112, r_0=1.0457$.

minimum, i.e., it is continuously attractive. Even without noise, there is no transition from rotation to translation, whereas the transition backwards stays unaffected. From this fact, we conclude that the existence of repulsive forces leads to a transition from rotation to translation.

To check this hypothesis, we approximate the Morse potential by a harmonic potential with equilibrium distance of the shape $U_{\text{app}}(r)=a(r-r_0)^2$, with $a=(\frac{l_r C_a}{l_a C_r})^{l_a/(l_a-l_r)} \frac{C_r}{2l_r} (\frac{1}{l_r}-\frac{1}{l_a})$ and $r_0=\frac{l_r l_a}{l_r - l_a} \ln \frac{l_r C_a}{l_a C_r}$, and compare it to the overall attractive harmonic potential $U_H(r)=ar^2$ (see Fig. 4). The critical noise value for the transition from translation to rotation is equal for the Morse potential and the harmonic approximation (not shown). The harmonic potential U_H is slightly more stable. The main difference occurs in the transition from rotation to translation. The harmonic approximation U_{app} shows this transition, though at a different noise value than the Morse potential. In the case of the harmonic potential U_H, the rotational mode is stable even without noise. This supports the assumption that a short-range repulsive part of the potential is vital for the existence of the transition from rotation to translation. For a plausible explanation, one might think of a Van-der-Waals gas as an analogy. There the attractive forces between molecules lead to the existence of a fluid or bound phase. Repulsive forces are treated as an effective volume that destabilizes the fluid phase. The same effect occurs when the temperature is increased, which can be interpreted as increasing the noise intensity. When we now identify the fluid phase with the translational mode and the gas phase with the rotational mode, the Van-der-Waals gas explains the role of repulsive forces for the transition from rotation to translation.

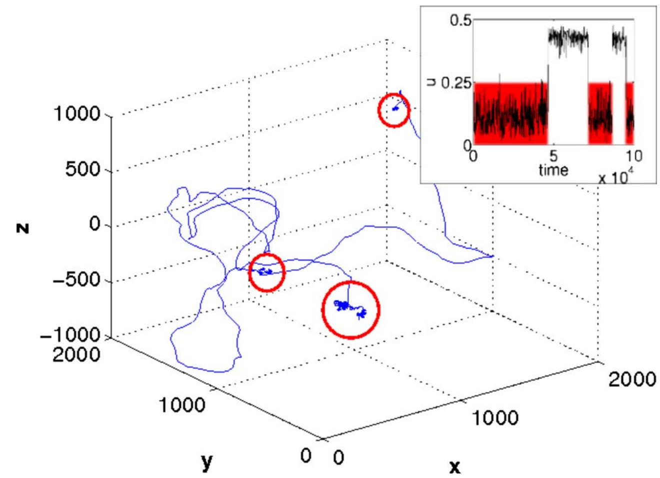

FIG. 5. (Color online) Example of a trajectory of the center of mass in the bistable regime. The inlay shows the corresponding velocity. The rotational modes where the velocity is almost zero are highlighted gray (red). These lead to a diffusive motion of the center of mass within the gray (red) circles. In between the system displays a stochastic trajectory in the translational mode with mean velocity $u \cong v_0 = \sqrt{\frac{\gamma_1}{\gamma_2}}$. Parameter values: $N=20, \gamma_1=0.5, \gamma_2=2.0, C_r=4.0, C_a=l_r=0.5, l_a=2.0, D=0.001\,25$.

C. Bistability

For both transitions, we observe the critical noise value to decrease with increasing amplitude of the repulsive part of the interaction potential C_r. Yet, the decrease is much faster for the transition from translation to rotation, which leads to a parameter region where transitions in both directions occur at the same noise value. In this region, the system alternates between the two states. The inset of Fig. 5 shows the center-of-mass velocity u, which alternates between translation and rotation (red). Figure 5 shows the trajectory of the center of mass. In between parts of ballistic motion, we see some spots where the system was rotating, which led to a diffusive motion of the center of mass. The probability distribution of u depends very sensitively on the noise intensity (Fig. 6). The region where this switching behavior can be observed is very small. Changing the noise value by a few percent leads to a shift of the transition probabilities, which is sufficient to destroy the switching.

IV. DIFFUSION OF THE ANGULAR MOMENTUM IN EXTERNAL POTENTIALS

A new effect that occurs in the three-dimensional case is the diffusion of the angular momentum. Since particles interacting via a Morse-type potential rotate coherently at low noise intensities, they have a nonzero mean angular momentum whose absolute value is fixed. In three dimensions, its direction diffuses. For an analytic approach, we need a simpler model that captures this property, and therefore we consider one particle in an external harmonic potential $U_H(\vec{r})=\frac{1}{2}\omega^2\vec{r}^2$. It is well known that this system possesses a stable solution corresponding to a circular motion with radius

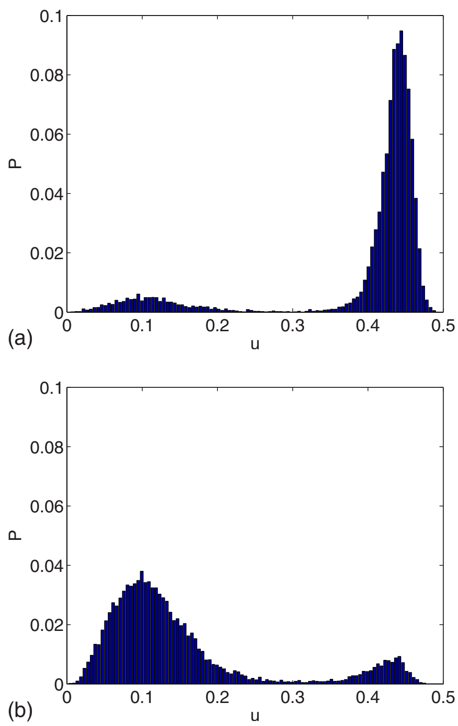

FIG. 6. (Color online) Probability distribution of the center-of-mass velocity for different noise values D. (a) $D=0.00115$, (b) $D=0.0013$. Other parameter values as in Fig. 5.

$r_0=\frac{v_0}{\omega}$ [29]. In the absence of noise, the angular momentum $\vec{L}=\vec{r}\times\vec{v}$ (remember that $m=1$) is fixed; the direction of motion depends on the initial conditions. In the two-dimensional case, the particle can rotate only clockwise or counterclockwise. Stochastic forces enable the particle to change its direction of rotation [30]. To do so, the particle has to cross a barrier of angular momentum [26]. In three dimensions, the particle moves on the surface of a sphere where it can rotate in any direction. When applying noise to the three-dimensional system, the direction of the angular momentum starts moving diffusively while its absolute value fluctuates around the noise-free value. As opposed to the two-dimensional case, the particle changes its direction of motion continuously; there is no barrier. For one particle in an external harmonic potential, we derive an analytical expression for the angular diffusion coefficient. This allows an estimation of the time a particle needs to turn its angular momentum.

To calculate this angular diffusion coefficient, we transform the equations of motion (6b) to a set of variables adapted to the spherical symmetry of the problem. The angular momentum is transformed to spherical coordinates where ϑ is the zenith angle and ϕ is the azimuth angle. This transformation and its solution for the noise-free deterministic case is shown in the Appendix. To obtain the diffusion coefficient of the angular momentum, we assume the velocity to be constant $v_0=\sqrt{\frac{\gamma_1}{\gamma_2}}$ and restrict the impact of noise to ϕ and ϑ. From this new set of differential equations, we obtain the Fokker-Planck equation,

$$\frac{\partial}{\partial t}P(\alpha,\beta,\vartheta,\phi) = -\omega\left(\frac{\partial}{\partial\alpha}+\frac{\partial}{\partial\beta}\right)P(\alpha,\beta,\vartheta,\phi) + \frac{D}{v_0^2}\left(\cos^2\beta\frac{\partial^2}{\partial\vartheta^2}+\sin^2\beta\frac{\partial^2}{\partial\phi^2} - \sin\beta\cos\beta\frac{\partial^2}{\partial\phi\partial\vartheta}\right)P(\alpha,\beta,\vartheta,\phi). \tag{13}$$

Here α and β denote the polar angles of $\vec{r}$ and $\vec{v}$, respectively, in the plane of movement. If the square root of the noise intensity $\sqrt{2D}$ is low compared to the potential energy $\omega^2 r$, the rotation of the particle will be much faster than the diffusion of the angular momentum. Therefore, we can average over the fast variable β and obtain

$$\frac{\partial}{\partial t}P(\alpha,\vartheta,\phi) = -\omega\frac{\partial}{\partial\alpha}P(\alpha,\vartheta,\phi) + \frac{D}{2v_0^2}\left(\frac{\partial^2}{\partial\vartheta^2}+\frac{\partial^2}{\partial\phi^2}\right)P(\alpha,\vartheta,\phi). \tag{14}$$

This yields the diffusion coefficient for the polar angle ϑ of the angular momentum for open boundary conditions

$$D_\vartheta = \frac{D}{2v_0^2} = \frac{D\gamma_2}{2\gamma_1}. \tag{15}$$

From Eq. (15), we infer the time the angular momentum needed to turn around an angle ϑ to be

$$\langle\vartheta^2\rangle = 2D_\vartheta t = \frac{\gamma_2}{\gamma_1}Dt. \tag{16}$$

To compare the three-dimensional system to the two-dimensional case, consider the case $L_z=0$. In two dimensions, this point has to be crossed as the angular momentum switches from positive to negative values when the particles change their direction of rotation. In three dimensions, this corresponds to $\langle\vartheta^2\rangle=(\frac{\pi}{2})^2$, since ϑ denotes the angle between $\vec{L}$ and the z axis. Inserting $\langle\vartheta^2\rangle=(\frac{\pi}{2})^2$ into Eq. (16) yields

$$t_{3d} = \frac{4\gamma_1}{\pi^2\gamma_2}\frac{1}{D}. \tag{17}$$

Setting $\gamma_1=5, \gamma_2=1$ we obtain $t_{3d}=\frac{2}{D}$ (see Fig. 7). In the two-dimensional system, the particle has to cross a barrier of the angular momentum in order to change its direction of rotation [29]. In the Kramers regime at low noise intensities, we expect the time to be proportional to an Arrhenius factor $t_{2d}\propto e^{\mathrm{const}/D}$ [31,32]. For higher noise intensities, this behavior passes to Einstein diffusion with the corresponding time $t\propto\frac{1}{D}$. This means that the diffusive motion of the angular momentum in three dimensions is faster than the switching in the two-dimensional case regardless of the noise intensity (see Fig. 7). We found the switching times to decrease with ω. Since ω does not appear in the Arrhenius factor, this points toward a complex forefactor depending on ω.

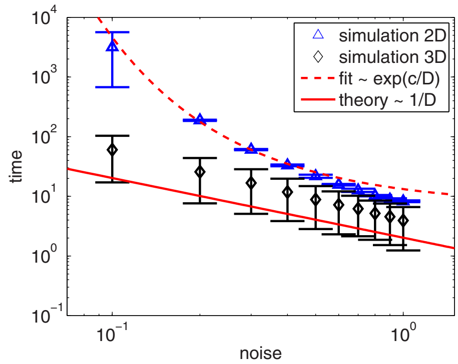

FIG. 7. (Color online) The figure displays the time needed for the angular momentum to turn around $\frac{\pi}{2}$ (3D [black, diamonds]) and the time needed for the angular momentum to switch between L_0 and 0 (2D [gray (blue), triangles]), respectively, versus noise intensity D for one particle in a harmonic potential, averaged over 1000 runs. In three dimensions, the time follows a power law (solid line). In two dimensions, we obtain an exponential correlation (dashed line) for low noise intensities that passes into a power-law behavior for higher noise intensities. Parameter values: $\gamma_1=5, \gamma_2=1, \omega=1$.

We now return to the system with many particles globally coupled by a Morse potential. Due to the asymmetry of the Morse-type potential, all particles will rotate in the same direction, leading to a torus shape structure (Fig. 2). Thus the average angular momentum equals approximately the angular momentum of each particle. Surprisingly, we find Eq. (16) to be still valid. However, in two dimensions the energy barrier separating the two rotational states grows with the number of particles, leading to an increase of the switching times. However, in the many-particle system, the diffusion of the angular momentum in three dimensions is always faster than the switching in two dimensions, too.

V. CONCLUSION

Active Brownian particles have been analyzed in a number of studies. It has been shown that in two dimensions, a set of particles interacting harmonically exhibits a noise-induced transition from translational to rotational motion. In this work, we investigated the extension to three spatial dimensions. Additionally, we considered an interaction via a Morse potential. For a harmonic interaction, the rotational mode is stable for any noise value. Applying a Morse-type interaction destabilizes the rotational motion and leads to a transition back to translational motion for low noise intensity. A harmonic interaction with equilibrium distance, i.e., with a repulsive part, also shows this back transition. This indicates that the existence of a repulsive force is vital for the transition back to translational motion. It is not yet clear how exactly the existence of a repulsive force destabilizes the rotational mode. This will be the subject of further studies. Moreover, this effect could not be observed in two dimensions. There the rotational motion was stable for all parameter values. In general, the transitions occur at different noise values, resulting in a hysteresis curve. We were able to find parameter regions where the transitions in both directions take place at the same noise value. Thus the system switches persistently between the two modes of motion.

One particle in an external harmonic potential exhibits a rotational motion. In two dimensions, it can rotate only clockwise or counterclockwise. Stochastic forces enable the particle to cross the barrier of the angular momentum and switch its direction. In three dimensions, the particle can change its direction of motion continuously. We derived an analytical expression of the diffusion coefficient of the angular momentum and showed that the change of the direction of motion is always faster in three dimensions.

ACKNOWLEDGMENTS

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APPENDIX

In the following, we will derive an analytic expression for the diffusion coefficient of the angular momentum of one particle moving actively in an external harmonic equation. Starting from the equations of motion (6b),

$$\dot{\vec{r}} = \vec{v}, \tag{A1a}$$

$$\dot{\vec{v}} = (\gamma_1 - \gamma_2 \vec{v}^2)\vec{v} - \omega^2 \vec{r} + \sqrt{2D}\vec{\xi}, \tag{A1b}$$

we will now choose a coordinate system adapted to the underlying symmetry of the problem. The particle is expected to move at a constant speed on a circle on the equipotential surface. The circle lies on a plane that is defined by the angular momentum. Under the influence of noise, the angular momentum moves diffusively in space while its absolute value fluctuates around its mean value. To describe this angular diffusion, we transform the system to coordinates adapted to the underlying symmetry of the problem.

We describe the angular momentum in spherical coordinates L, ϑ, and ϕ where

$$\vec{L} = L(\sin\vartheta\cos\phi, \sin\vartheta\sin\phi, \cos\vartheta)$$

(see Fig. 8). The plane perpendicular to $\vec{L}$ is the plane of movement. Let us call the intersection of this plane with the x-y plane the node line. Then the angle α between this node line and $\vec{r}$ defines the position of $\vec{r}$ on this plane. The angle β is defined analogously as the angle between the node line and $\vec{v}$. The last two variables r and v are the absolute values of $\vec{r}$ and of $\vec{v}$.

Introducing the unity vector in direction of $\vec{L}$, $\vec{e}_L$, we can transform the differential equations for $\vec{r}$ and $\vec{v}$ into differential equations of our new variables and obtain in Stratonovich interpretation

$$\dot{r} = v\cos(\alpha - \beta), \tag{A2}$$

$$\dot{v} = (\gamma_1 - \gamma_2 v^2)v - \omega^2 r\cos(\alpha-\beta) + \frac{\sqrt{2D}}{v}\vec{v}\cdot\vec{\xi}, \tag{A3}$$

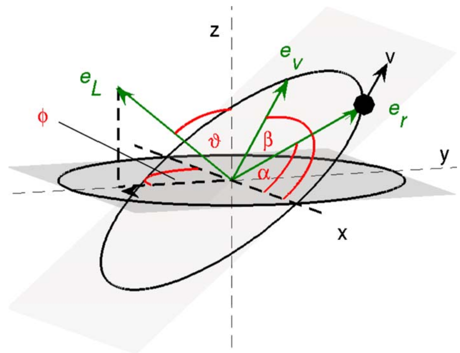

FIG. 8. (Color online) Spherical coordinate system. The shaded planes are the x-y plane (dark gray) and the plane of movement (light gray). Their intersection, in this case the x axis, is called the node line. $\hat{e}_r$ is the unit vector in space, $\hat{e}_v$ in velocity, and $\hat{e}_L$ in the angular momentum. The angle between $\hat{e}_r$ and the node line is called α, the one between $\hat{e}_v$ and the node line is called β. ϑ and ϕ are the common angles of the angular momentum in polar coordinates, i.e., ϑ is the angle between $\hat{e}_L$ and the z axis and ϕ is the angle between the projection of $\hat{e}_L$ on the x-y plane and the x axis.

$$\dot{\alpha} = (\gamma_1 - \gamma_2 v^2) v \cot \alpha + \omega^2 \frac{r \cos \beta}{v \sin \alpha} + \frac{\sqrt{2D}}{v}\left[\frac{\sin \phi \sin \vartheta}{\cos \vartheta \sin(\alpha - \beta)} \vec{e}_L \cdot \vec{\xi} + \frac{L}{\sin \alpha}(\cos \phi \xi_y - \sin \phi \xi_x)\right], \tag{A4}$$

$$\dot{\beta} = -\frac{v \cos \alpha}{r \sin \beta} + \frac{\sqrt{2D}}{v}\frac{\sin \beta \sin \vartheta}{\sin(\alpha - \beta)} \vec{e}_L \cdot \vec{\xi}, \tag{A5}$$

$$\dot{\phi} = \frac{\sqrt{2D}}{v}\frac{\sin \beta}{\sin(\alpha - \beta)} \vec{e}_L \cdot \vec{\xi}, \tag{A6}$$

$$\dot{\vartheta} = \frac{\sqrt{2D}}{v}\frac{\cos \beta}{\sin(\alpha - \beta)} \vec{e}_L \cdot \vec{\xi}. \tag{A7}$$

First we will consider the deterministic noise-free case. Then we get $\dot{\phi}=0$ and $\dot{\vartheta}=0$. So the motion of our particle is fixed on a plane and therefore reduced to four variables,

$$\dot{r} = v \cos(\alpha - \beta), \tag{A8}$$

$$\dot{v} = (\gamma_1 - \gamma_2 v^2) v - \omega^2 r, \tag{A9}$$

$$\dot{\alpha} = (\gamma_1 - \gamma_2 v^2) v \cot \alpha + \omega^2 \frac{r \cos \beta}{v \sin \alpha}, \tag{A10}$$

$$\dot{\beta} = -\frac{v \cos \alpha}{r \sin \beta}. \tag{A11}$$

This system possesses two solutions with $\dot{r}=0$ and $\dot{v}=0$. The trivial solution $r_1=v_1=0$ is unstable. α and β are not defined in this case since $\vec{r}_1=0$ and $\vec{v}_1=0$. The stable solution reads $r_2=\frac{v_2}{\omega}$, $v_2=\sqrt{\frac{\gamma_1}{\gamma_2}}$, $\cos(\alpha_2-\beta_2)=0 \Rightarrow \alpha_2-\beta_2=\pm\pi/2$ with stationary angular velocity $\dot{\alpha}_2=\dot{\beta}_2=\pm\omega$.

To calculate the diffusion coefficient of the angular momentum, we have to leave the deterministic case and include noise. In first approximation, we consider a stationary velocity and angular velocity, which are set to the stable solutions of the deterministic case $v_0=v_2=\sqrt{\frac{\gamma_1}{\gamma_2}}$ and $r_0=r_2=\frac{v_2}{\omega}$, respectively. This yields

$$\dot{r}_0 = 0, \tag{A12}$$

$$\dot{v}_0 = 0, \tag{A13}$$

$$\dot{\alpha} = \omega, \tag{A14}$$

$$\dot{\beta} = \omega, \tag{A15}$$

$$\dot{\phi} = \frac{\sqrt{2D}}{v_0}\frac{\sin \beta}{\sin(\alpha - \beta)} \vec{e}_L \cdot \vec{\xi}, \tag{A16}$$

$$\dot{\vartheta} = \frac{\sqrt{2D}}{v_0}\frac{\cos \beta}{\sin(\alpha - \beta)} \vec{e}_L \cdot \vec{\xi}. \tag{A17}$$

The corresponding Fokker-Planck equation reads

$$\frac{\partial}{\partial t}P(\alpha,\beta,\vartheta,\phi) = -\omega\left(\frac{\partial}{\partial \alpha} + \frac{\partial}{\partial \beta}\right)P(\alpha,\beta,\vartheta,\phi) + \frac{D}{v_0^2}\left(\cos^2 \beta \frac{\partial^2}{\partial \vartheta^2} + \sin^2 \beta \frac{\partial^2}{\partial \phi^2} - \sin \beta \cos \beta \frac{\partial^2}{\partial \phi \partial \vartheta}\right)P(\alpha,\beta,\vartheta,\phi). \tag{A18}$$

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