Run-and-Tumble Dynamics of Self-Propelled Particles in Confine-
ment

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PACS 82.70.-y – Disperse systems; complex fluids
PACS 45.50.-j – Dynamics and kinematics of a particle and a system of particles
PACS 05.40.-a – Fluctuation phenomena, random processes, noise, and Brownian motion

Abstract – Run-and-tumble dynamics is a wide-spread mechanism of swimming bacteria. The
accumulation of run-and-tumble microswimmers near impermeable surfaces is studied theoretically
and numerically in the low-density limit in two and three spatial dimensions. Both uni-modal and
exponential distributions of the run lengths are considered. Constant run lengths lead to peaks
and depletions regions in the density distribution of particles near the surface, in contrast to
exponentially-distributed run lengths. Finally, we present a universal accumulation law for large
channel widths, which applies not only to run-and-tumble swimmers, but also to many other kinds
of self-propelled particles.

Introduction. – Swimming bacteria like E. coli and Salmonella, with a body length of just a few micrometers,
are too small for spatial sensing of a stimulus gradient along their body size [1,2]. Therefore, they have to re-
sort to temporal sensing, where the gradient is determined along the swimming trajectory. These bacteria have de-
veloped a procedure of intriguing simplicity for chemotac-
tic motion — they perform a run-and-tumble motion, in
which nearly straight swimming segments are interrupted
by tumbling events, where the run length then depends
on the sign of the stimulus gradient [1,3]. There is an in-
teresting connection of this run-and-tumble dynamics to
Lévy flights [4,5], which suggests that this process could
be a very efficient search strategy [6].

For a dilute suspension of microswimmers in a bulk
fluid, run-and-tumble dynamics is strictly equivalent to
passive-particle diffusion for long times. Here, the dif-
fusion coefficient is given by $D_{\text{eff}} = \frac{v^2}{\tau_r}$, where $v$ is the
swimming velocity, and $\tau_r$ is the run time [7]. The effec-
tive diffusion coefficient is typically much larger than the
thermal diffusion coefficient. The equivalence also holds in
the presence of a slowly varying external potential. This
implies that active Brownian particles (ABPs), which dis-
play a rotational diffusion instead of tumbling events, are
equivalent to run-and-tumble particles (RTPs) under these
conditions.

In fact, the equivalence of ABPs and RTPs has been
discovered much earlier for the mathematically equivalent
case of the conformations of semi-flexible polymers. Here,
the worm-like chain model corresponds to ABPs, whereas
the freely-jointed chain model corresponds to RTPs. The
equivalence of the two is expressed by the Kuhn length
$\xi_K$, which is the segment length of the freely-jointed chain,
to equal twice the persistence length $\xi_p$ of the worm-like
chain, such that the end-to-end distance is the same in
both descriptions [8].

At higher densities of microswimmers, a density-
dependent motility can cause phase separation and ac-
cumulation of both RTPs [9,11] and ABPs [12,14], which
indicates that the dynamics of active particles is no longer
equivalent to passive diffusion. Asymmetric potentials can
cause rectification of bacterial motion [7,15,16]. Also,
walls and obstacles break the diffusion equivalence, be-
cause microswimmers accumulate at walls, in contrast to
passive particles. Explanations of this surface trapping
usually invoke hydrodynamics [17,18]. Whether it is the
detailed hydrodynamics of the corkscrew motion of E. coli
flagella [19] or the snake-like motion of the sperm tail [20],
or the far-field hydrodynamics of a hydrodynamic dipole
[17], hydrodynamics provides an effective attraction to-
ward boundaries [18,21,22]. However, for E. coli, noise
also plays an important role and may even dominate over
the rather weak hydrodynamic interactions [23]. Further-
more, it has been shown that persistent motion drives
swimmers to the wall, even in presence of strong orientational fluctuations \[24\] \[29\]. For harmonic confinement, accumulation away from the center has also been found for run-and-tumble particles \[7\]. Thus, it is not obvious under which conditions the equivalence between RTPs, ATPs, and passively diffusing particles holds. We want to clarify this question from the point of view of wall accumulation and confinement.

In this letter, we investigate the effect of confinement for particles with a pure run-and-tumble dynamics in the low-density limit and in the absence of hydrodynamic interactions, both analytically and numerically. The structure of the density patterns of RTPs at hard walls is found to depend strongly on the dimensionality of the accessible space — between two planar walls in three dimensions (3D), or along a surface with lateral confinement in two dimensions (2D) — and on the run-length distribution, both quantitatively and qualitatively. Here, the relevant parameter is the dimensionless ratio between channel width and (average) run length, whereas propulsion velocity and tumbling frequency only enter indirectly via the run length. RTPs are predicted to behave quite differently from ABPs. For narrow channels and constant run lengths, the distribution of tumbling events develops pronounced extrema, with a depletion layer near the wall and a maximum at larger distances determined by the run length. These structures disappear for exponentially distributed run lengths. Thus, the behavior depends sensitively on the run-length distribution. In contrast, for wide channels, we predict a (nearly) universal wall-accumulation law for self-propelled particles. This wall-accumulation law only relies on symmetries and dimensional arguments, and thus holds for many different types of microscopic swimmers.

Wild-type E. coli have an average run length of \(12 \mu\text{m} \[30\]\), which is the same order of magnitude as the channel width of microfluidic devices used to manipulate and study these bacteria \[31\] \[33\]. Therefore, our results are relevant, inter alia, for the design of microfluidic devices for rectification and sorting of run-and-tumble bacteria.

Model and Simulation Technique. – We study run-and-tumble dynamics of individual microswimmers in confinement. A particle performs a forward run with a velocity \(v\) for a time \(\tau_r\). Each run is followed by a tumble event, where a new orientation angle \(\theta\) (see Fig. 1) is chosen randomly on the unit circle (2D) or unit sphere (3D), i.e. there is no memory of the orientation before the tumbling event. The particle coordinate \(z\) perpendicular to the wall is then updated by \(z(t + \tau_r) = z(t) + \cos(\theta)L\). Here, the run length \(L = v\tau_r\) is either constant, or drawn from an exponential distribution depending on the dynamics studied. It is important to note that properties of RTPs do not depend on \(v\) and \(\tau_r\) separately, but only on the run length. Due to symmetry, motion parallel to the wall does not have to be considered. If the particle hits a wall, it remains there – possibly sliding parallel to the wall – until the next tumbling event occurs. After a sufficiently long equilibration time, the probability density to find the particle at a position \(z\) is recorded by a histogram over \(10^8\) to \(10^9\) tumbling steps. A few examples of density distributions for various run lengths are shown in Fig. 2.

The trajectory of an RTP is completely defined by the location of the tumbling events, since the motion between these events is just ballistic. This implies, in particular, that no orientation vector of the particle is needed to describe the dynamics. Thus, the continuous-time dynamics of a RTP in three spatial and two orientational dimensions is mapped onto a discrete-time-step model in one spatial dimension. Physically and mathematically, the fundamental quantity to compute in the steady state is then the tumbling density \(\phi(z)\). The particle density \(\rho(z)\) then follows from \(\phi(z)\) by a convolution, as explained in detail below. Both densities are directly accessible experimentally; however, the tumbling density is more difficult to measure, because the trajectories of (all) particles have to be traced.

Thus, we first focus on the more fundamental tumbling density, which is the (normalized) probability to find a tumbling event at a position \(z\). The mirror symmetry of the system is reflected in the symmetry of the tumbling density, \(\phi(z) = \phi(-z)\). The time evolution of the tumbling density is determined by

\[
\frac{\partial}{\partial t} \phi(z, t + \tau_r) = \int_{-d}^{d} \phi(z', t)p(z - z')dz'.
\]

Fig. 1: Schematic of run-and-tumble dynamics. A “run” of the particle with a velocity \(v\) for a time \(\tau_r\) is followed by a tumbling event, resulting in a new orientation \(\theta\). The particle is confined between two parallel walls at \(z = \pm d\). \(z^*\) denotes the distance from the walls.

Here, \(p(\Delta z)\) is the transfer function of particles moving to a new position, which depends implicitly on the run-length distribution. It is the number of orientational microstates of an unconfined particle which are compatible with a given \(\Delta z\)-displacement. This probability density depends on the dimensionality of the system, and on the run length distribution (unimodal or exponentially distributed). At the walls, particles accumulate in a \(\delta\)-distribution because all particles that hit the wall are located there. Thus, we have
the boundary conditions

\[ \phi(\pm d, t) = 0.5 \phi_s(t) \delta(z \pm d) \]  \hspace{1cm} (2)

\[ 0.5 \phi_s(t + \tau_r) = \int_{-d}^{d} \phi(z', t) P(-z' - d) dz' \]  \hspace{1cm} (3)

where \( \phi_s \) is the probability to find a tumbling event at the wall, and \( P \) is the cumulative distribution function of \( \rho \), i.e. \( P(z) = \int_{-\infty}^{z} p(z') dz' \).

**Constant Run Lengths.** – We begin our analysis in the simplest case of constant run length \( L \). The transfer function is discontinuous at the run length, as runs longer than \( L \) cannot occur. In three dimensions, the transfer function \( p(z)dz \) is obtained by an integral over the surface of a sphere of radius \( L \) with values of the vertical displacement between \( z \) and \( z + dz \). This yields immediately that the transfer function is

\[ p_{(3,c)}(z) = \frac{1}{2L} \Theta(L - z) \Theta(L + z), \]  \hspace{1cm} (4)

where \( \Theta(z) \) is the Heaviside step function. Subscripts denote dimensionality and the type of run length distribution (\( c=\)constant, \( e=\)exponential). Similarly, in two dimensions, integration over a circle of radius \( L \) with displacement between \( z \) and \( z + dz \) yields even a divergence of the transfer function at the run length,

\[ p_{(2,c)}(z) = \frac{1}{\pi L \sqrt{1 - (z/L)^2}} \Theta(L - z) \Theta(L + z). \]  \hspace{1cm} (5)

The simplicity of the 3D transfer function allows for an analytic solution for narrow channels with \( 2d < L \),

\[ \phi_{(3,c)}(z) = \frac{1}{2L} + \frac{d/L}{2} [\delta(z - d) + \delta(z + d)] \]  \hspace{1cm} (6)

In 2D, an analytical solution can only be obtained by assuming that the number of tumbling events in the bulk is negligible compared to tumbling events at the wall (i.e. with \( \Delta z = z \) cannot be achieved with \( L' < z \).

We focus here on exponential run length distributions,

\[ p_{cen}(L') = \lambda \exp(-\lambda L'), \]  \hspace{1cm} (9)

with \( \langle L' \rangle \equiv L = 1/\lambda \), which mimic the run-length distribution of *E. coli*. This yields the transfer functions

\[ p_{(2,e)}(z) = \frac{1}{\pi L} K_0 \left( \frac{|z|}{L} \right), \]

\[ p_{(3,e)}(z) = \frac{1}{2L} E_1 \left( \frac{|z|}{L} \right) \]  \hspace{1cm} (10)

These analytical results and corresponding simulation data are displayed in Fig. [3]. The comparison shows that the solution \([6]\) in 3D and the approximate expression \([7]\) in 2D work very well for the appropriate regimes. Figure [3] reveals that the walls induce a very rich structure of the tumbling density in the channel for \( 2d \geq L \), i.e. for channels wider than the run length. The density profiles all collapse onto a single master curve when the tumbling density is scaled by the bulk density \( \phi_b \) (the density far away from the wall) and distances are scaled by the run length. In this case, the high particle density at the walls generates depletion regions near the walls, and two pronounced peaks at a distance \( L \) from the wall, which can easily be recognized in Fig. [3] (middle) and (right). In 2D, these primary peaks generate secondary peaks for \( d \geq L \), which are again displaced by a distance \( L \) further away from wall they first came from. In 3D, the primary singularities are too weak to generate visible secondary peaks. All bulk singularities disappear for \( L > 2d \), compare Eq. \([6]\), because particles can move directly from one wall to the other in a single step. These depletion zones and peaks can be understood by starting from a uniform bulk distribution plus \( \delta \)-peaks at the walls, and iterating Eq. \([1]\) once, as explained in more detail below.

**Exponential Run-Length Distribution.** – In the case of a distribution of run lengths, the transfer functions are obtained by convolution of the (conditional) probabilities \( p(z|L') \) — resulting from step with run length \( L' \) — with the run-length distribution \( p_{cen}(L') \), i.e.

\[ p_{(n,cen)}(z) = \int_{L}^{\infty} P_{(n,c)}(z|L') p_{cen}(L') dL' \]  \hspace{1cm} (8)

The integral has a lower boundary at \( z \), because \( \Delta z = z \) cannot be achieved with \( L' < z \).

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Scaling Behavior of Wall Density. — For channels much wider than the (average) run length, we can use scaling arguments to determine the wall accumulation of particles. For \(d \gg L\), the tumbling density profile eventually becomes flat far from the walls. Everything else fixed, the surface density has to be linear in the bulk density \(\phi_b\) defined as the (constant) density far from the walls. Since the (average) run length \(L\) is the only relevant length scale near the wall, the proportionality factor has to be linear in \(L\), so that

\[\phi_s = \alpha L \phi_b\]

with a dimensionless prefactor \(\alpha\). In a channel of finite width \(d\), normalization then gives

\[\phi_s = \frac{\alpha L}{\alpha L + 2d} = \frac{1}{1 + 2d/(\alpha L)}.\]

The surface accumulation factor \(\alpha\) is independent of run length, and only depends on the dynamics (i.e. 2D/3D, 4D). Alternatively, it can be argued that the surface density \(\phi_s\), which is dimensionless in our description, can only depend on the ratio of the two available length scales \(L\) and \(d\), which implies \(\phi_s = F(d/L)\), with some unknown scaling function \(F(x)\). This can also be seen by considering an infinite half-space, with a wall at \(z = 0\). In this case, the boundary condition is that the density approaches \(\phi_b\) for \(z \to \infty\). Then, \(L\) is the only available length scale. For finite but very wide channel, the density profile should not change. However, the normalization of the probability density introduces a constraint on \(\phi_b\), which implies \(\phi_b \sim 1/d\).
constant run length/ exponential run-length distribution). From our simulations, we obtain the accumulation factors shown in Table 1. The large-distance approximation \[14\] works very well for \(d > L\), and even for smaller channels it is not too far off (see Fig. 3). Unimodal and exponential run-length distributions result in accumulation factors \(\alpha\), which are clearly different, but still of the same order of magnitude. Thus, measurements of \(\alpha \equiv \phi_s/(L\phi_b)\) for \(d \gg L\) might provide a new possibility to characterize run-length distributions experimentally.

Since these arguments rely only on dimensional analysis, the results should be valid for other types of self-propelled particles as well (as long as there is one dominant length scale of the dynamics). For active Brownian spheres, this length scale is the persistence length of the trajectory \(\xi_p = v/D_r\), where \(D_r\) is the rotational diffusion coefficient. Using data from Ref. \[26\], we find indeed an excellent agreement for channels much larger than the diffusive length scale \(l_D = \sqrt{D_r/D_c}\) (see Fig. 4). Note that Eq. \[14\] also predicts a crossover from narrow- to wide-channel behavior at \(L \simeq 2d\) for all kinds of self-propelled particles. The fact that the \(\alpha\)-values in Table 1 differ significantly for RTPs and ABPs clearly demonstrates that these two types of self-propelled motion are not equivalent near surfaces. However, the fact that these factors are all of order one emphasizes the generic aspect of wall accumulation.

### Near-Wall Density in Wide Channels.

For wider channels, the surface density \(\phi_s\) is well described by Eq. \[14\]. To understand the structure of the density distribution close to the wall, the stationary form of Eqs. \(1\) to \(3\) can be used to obtain an analytical approximation. We start as an initial guess with a \(\delta\)-distribution at the wall, with an amplitude \(\phi_b\), plus a constant tumbling density \(\phi_s\) in the bulk (see Eq. \[14\]). An iteration with Eq. \(1\) then yields

\[
\phi_1(z^*) = \frac{\phi_s}{4} \delta(z^*) + \phi_b \delta(z^*) \int_0^\infty P(z')dz' + \frac{\phi_s}{2} P(z^*) + \phi_b \left(1 - \int_0^\infty p(z^* - z')dz'\right). \tag{15}\]

Note that the last two terms on the right-hand side of Eq. \[15\] determine the spatial dependence of the tumbling density near the wall. Figure 3 (center) shows that this first-order calculation can qualitatively explain the numerical results for the structure of the tumbling-density profile. In particular, for constant run lengths, it reproduces and explains the near-wall dip in the tumbling density, i.e. the formation of a depletion layer close to the wall, and in turn a peak and discontinuity at \(z = L\). As shown in Fig. 3 (right), this peak leads to interesting patterns in the tumbling-density distribution for channel widths larger than the run length, in particular a very pronounced peak in the channel center for \(d = L\).

### Microswimmer Density.

Finally, we connect the tumbling density to the number density of microswimmers. This requires the convolution of the tumbling density with the spreading function \(f(\Delta z)\) of one run,

\[
\rho(z) = \int_{-\infty}^{\infty} \phi(z') f(z - z') dz' \tag{16}\]

(where the particles which would penetrate the walls have to be "folded back" to the wall, i.e. \(\phi_s(d) = \int_d^\infty P(z)dz\)). For constant run length, the spreading function \(f(\Delta z)\) is obtained from the transfer functions as

\[
f(z) = \int_z^{\infty} p(z) \frac{dz'}{z'} \tag{17}\]

and \(z < 0\) follows from symmetry.\(^2\) Note that if the tumbling time \(\tau_t\) cannot be neglected compared to the run time \(\tau_r\), the tumbling density has to be added proportional to \(\tau_t/\tau_r\) in Eq. \[16\]. As an example, we consider here the case of thin three-dimensional channels \((2d < L)\) and constant run length, which can be solved analytically. Here, the spreading function is found to be

\[
f(z) = \frac{1}{2L} \ln \left(\frac{L}{z}\right), \tag{18}\]

\(^2\)In the more general case, Eq. \[17\] has to be modified to account for the run-length distribution.
which yields the particle density (for $z > 0$)

$$
\rho(z) = \frac{1}{4\pi} \left[ \ln \left( \frac{L}{d + z} \right) + \ln \left( \frac{L}{d - z} \right) \right] \\
+ \frac{d}{4\pi z^2} \left[ 2 + \frac{z}{d} \ln \left( \frac{d - z}{d + z} \right) \right] \\
+ \frac{\rho_s}{2} \delta(z - d) + \frac{\rho_s}{2} \delta(z + d)
$$

(19)

where the surface density $\rho_s$ of particles is obtained from the normalization condition. Equation (19) fits the simulations perfectly, without any adjustable parameters, see Fig. 2.

Conclusions. – We have shown that run-and-tumble dynamics of self-propelled particles leads to highly structured density distributions near impenetrable surfaces. Due to the absence of translational diffusion, accumulation materializes in the form of $\delta$-function peaks at the surface. Diffusion would broaden these peaks, similarly as predicted for ABPs [26]. Close to confining walls, RTPs are thus clearly not equivalent to either diffusing particles or ABPs. The density distributions are predicted to depend sensitively on the spatial dimensionality and on the run-length distribution, where the typical length scale is set by the (average) run length.

While the dynamics considered here is certainly over-simplified for real microswimmers like E. coli, it captures the essential aspects of run-and-tumble motion, and similar results can be expected for other types of Levy flights. In particular, the limit of large wall separations for the accumulation is very generic, and should thus apply to many systems of self-propelled particles and microswimmers [21][22]. It will be interesting to see whether this behavior extends to systems in which hydrodynamic interactions play a significant role.

Another interesting issue is the behavior of RTPs at finite particle density [9][11]. For high density, the characteristic features in confinement revealed by our study will almost certainly be washed out, because collisions will dominate over tumbling events. However, interesting behavior can be expected in confinement, when the average distance between particles becomes comparable with the run length.

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