Reynolds numbers

\[ Re = \frac{\rho UL}{\mu} = \frac{UL}{\nu} \]
E. coli (non-tumbling HCB 437)

Drescher, Dunkel, Ganguly, Cisneros, Goldstein (2011) PNAS
Bacterial motors

movie: V. Kantsler

Chen et al (2011) EMBO Journal

~20 parts

source: wiki
Chlamy


dunkel@math.mit.edu
Eukaryotic motors

Sketch: dynein molecule carrying cargo down a microtubule

http://www.plantphysiol.org/content/127/4/1500/F4.expansion.html

Yildiz lab, Berkeley
Microtubule filament “tracks”

Drosophila oocyte

Physical parameters (e.g. bending rigidity) from fluctuation analysis
Unlike dyneins, (most) kinesins walk towards the plus end of the microtubule.
Kinesin walks hand-over-hand

Yildiz et al (2005) Science
Kinesin walks hand-over-hand

Yildiz et al (2005) Science
Intracellular transport

Chara corralina

http://damtp.cam.ac.uk/user/gold/movies.html
Muscular contractions: Actin + Myosin

G-Actin (globular)

F-Actin helical filament
Actin-Myosin

Myosin

F-Actin
helical filament
Actin-Myosin

Myosin

F-Actin helical filament

myosin-II

myosin-V

processive movement of myosin V along F-actin
Myosin walks hand-over-hand

Hand over hand

Catalytic domain
Cargo binding domain
Light chain domain

Inchworm

37 nm
74 nm
37 nm
37 nm - 2x
74 nm
37 nm
37 nm + 2x
37 nm
37 nm
37 nm
37 nm
37 nm
37 nm
37 nm

A 37 nm  A'  A'

B 37 nm  B  B

Fig. 3. Stepping traces of three different myosin V molecules displaying 74-nm steps and histogram (inset) of a total of 32 myosin V's taking 231 steps. Calculation of the standard deviation of step sizes can be found (14). Traces are for BR-labeled myosin V unless noted as Cy3 Myosin V. Lower right right trace, see Movie S1.

Bacteria-driven motor

Di Leonardo (2010) PNAS
Feynman-Smoluchowski ratchet
generic model of a micro-motor
Basic ingredients for rectification

- some form of noise (not necessarily thermal)
- some form of nonlinear interaction potential
- spatial symmetry breaking
- non-equilibrium (broken detailed balance) due to presence of external bias, energy input, periodic forcing, memory, etc.
Eukaryotic motors

Sketch: dynein molecule carrying cargo down a microtubule

http://www.plantphysiol.org/content/127/4/1500/F4.expansion.html

Yildiz lab, Berkeley
Adopting these rates and considering the asymptotic limit $t \to 1$, one can Taylor-expand the exact solution (1.112) for $Ax^\ast\tau D$ to obtain
\begin{equation}
\mathbb{P} \left( \pm (t) \right) = k K \cdot 1 \pm Ax^\ast D \cos(\beta t) + \mathcal{K} (\pm Ax^\ast D) \cos^2(\beta t) \pm \ldots
\end{equation}
(1.114)
These approximations are valid for slow driving (adiabatic regime), and they allow us to compute expectation values to leading order in $Ax^\ast D$. In particular, one then finds for the mean position the asymptotic linear response result [GHJM98]
\begin{equation}
E\left[ X(t) \right] = X \cos(\beta t) \quad (1.115 a)
\end{equation}
where
\begin{equation}
X = \frac{Ax^2 \mathcal{K} \beta}{4 k^2 K^4} + \beta^2 \quad (1.115 b)
\end{equation}
with $k K$ denoting Kramers rate as defined in Eq. (1.91). Note that Eqs. (1.115) are consistent with our earlier result (1.107).

1.6 Brownian motors
Many biophysical processes, from muscular contractions to self-propulsion of microorganisms or intracellular transport, rely on biological motors. These are, roughly speaking, collections of proteins that are capable of rectifying thermal and other random fluctuations to achieve directed motion. Here, we focus on a minimal mathematical model that captures, in a simplified manner, the main building principles of Brownian motors:
\begin{itemize}
  \item as spatially periodic structure (ratchet potential) that violates symmetry,
  \item thermal or non-thermal random fluctuations, and
  \item adequate deterministic to stochastic pumping processes that drive the system away from thermal equilibrium.
\end{itemize}
Generally speaking, the combination of broken spatial symmetry and non-equilibrium driving is sufficient for generating stationary currents by means of a ratchet effect.

Most biological micro-motors operate in the low Reynolds number regime, where inertia is negligible. A minimal model can therefore be formulated in terms of an over-damped Ito-SDE
\begin{equation}
dX(t) = -U'(X) dt + F(t) dt + \sqrt{2D(t)} dB(t).
\end{equation}
(1.116)

For further reading, we refer to the review articles [HM09, Rei02].
Most biological micro-motors operate in the low Reynolds number regime, where inertia is negligible. A minimal model can therefore be formulated in terms of an over-damped Ito-SDE

\[ dX(t) = -U'(X) dt + F(t) dt + \sqrt{2D(t)} \, dB(t). \]  

(1.116)

Here, \( U \) is a periodic potential

\[ U(x) = U(x + L) \]  

(1.117a)

with broken reflection symmetry, i.e., there is no \( \delta x \) such that

\[ U(-x) = U(x + \delta x). \]  

(1.117b)
Most biological micro-motors operate in the low Reynolds number regime, where inertia is negligible. A minimal model can therefore be formulated in terms of an over-damped Ito-SDE

\[
\frac{dX(t)}{dt} = -U'(X) dt + F(t) dt + \sqrt{2D(t)} \cdot dB(t).
\]

(1.116)

Here, \( U \) is a periodic potential

\[
U(x) = U(x + L)
\]

(1.117a)

with broken reflection symmetry, i.e., there is no \( \delta x \) such that

\[
U(-x) = U(x + \delta x).
\]

(1.117b)

A typical example is

\[
U = U_0[\sin(2\pi x/L) + \frac{1}{4}\sin(4\pi x/L)].
\]

(1.117c)

The function \( F(t) \) is a deterministic driving force, and the noise amplitude \( D(t) \) can be time-dependent as well.
Fig. 2.2. Typical example of a ratchet-potential $V(x)$, periodic in space with period $L$ and with broken spatial symmetry. Plotted is the example from (2.3) in dimensionless units.
The corresponding FPE for the associated PDF $p(t, x)$ reads

$$\partial_t p = -\partial_x j, \quad j(t, x) = -\{[U' - F(t)]p + D(t)\partial_x p\}, \quad (1.118)$$

and we assume that $p$ is normalized to the total number of particles, i.e.

$$N_L(t) = \int_0^L dx \, p(t, x) \quad (1.119)$$

gives the number of particles in $[0, L]$. The quantity of interest is the mean particle velocity $v_L$ per period defined by

$$v_L(t) := \frac{1}{N_L(t)} \int_0^L dx \, j(t, x). \quad (1.120)$$
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$$\partial_t p = -\partial_x j, \quad j(t, x) = -\{[U' - F(t)]p + D(t)\partial_x p\},$$

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$$N_L(t) = \int_0^L dx \, p(t, x)$$

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$$v_L(t) := \frac{1}{N_L(t)} \int_0^L dx \, j(t, x).$$

(1.120)

Inserting the expression for $j$, we find for spatially periodic solutions with $p(t, x) = p(t, x + L)$ that

$$v_L = \frac{1}{N_L(t)} \int_0^L dx \, [F(t) - U'(x)] \, p(t, x).$$

(1.121)
1.6.1 Tilted Smoluchowski-Feynman ratchet

As a first example, assume that $F = \text{const.}$ and $D = \text{const.}$ This case can be considered as a (very) simple model for kinesin or dynein walking along a polar microtubule, with the constant force $F \geq 0$ accounting for the polarity. We would like to determine the mean transport velocity $v_L$ for this model.

To evaluate Eq. (1.121), we focus on the long-time limit, noting that a stationary solution $p_\infty(x)$ of the corresponding FPE (1.118) must yield a constant current-density $j_\infty$, i.e.,

$$j_\infty = -[(\partial_x \Phi)p_\infty + D\partial_x p_\infty]$$

(1.122)

where

$$\Phi(x) = U(x) - xF$$

(1.123)
1.6.1 Tilted Smoluchowski-Feynman ratchet

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$$j_\infty = -[(\partial_x \Phi)p_\infty + D \partial_x p_\infty]$$

(1.122)

where

$$\Phi(x) = U(x) - xF$$

(1.123)

is the full effective potential acting on the walker. By comparing with (1.85), one finds that the desired constant-current solution is given by

$$p_\infty(x) = \frac{1}{Z} e^{-\Phi(x)/D} \int_x^{x+L} dy \ e^{\Phi(y)/D}.$$  

(1.124)
As a first example, assume that

Here, to evaluate Eq. (1.121), we focus on the long-time limit, noting that a stationary \( p_1(x) \) of the corresponding FPE (1.118) must yield a constant current-density \( \partial_t \Phi \) for the polarity. We would like to determine the mean particle velocity \( v_1(x) \), \( j_\infty = -[(\partial_x \Phi)p_\infty + D\partial_x p_\infty] \)

\[
v_1(t) := \frac{1}{N_L(t)} \int_0^L dx \, j(t, x) = \frac{1}{N_L(t)} \int_0^L dx \, [F(t) - U'(x)] \, p(t, x) \quad j_\infty = -[(\partial_x \Phi)p_\infty + D\partial_x p_\infty]
\]

where we have used the coordinate transformation \( z = y - L \in [x, x + L] \) after the first line.

\[
p_\infty(x) = \frac{1}{Z} e^{\Phi(x)/D} \int_x^{x+L} dy \, e^{\Phi(y)/D}. \tag{1.124}
\]

This solution is spatially periodic, as can be seen from

\[
p_\infty(x + L) = \frac{1}{Z} e^{-[U(x+L)-(x+L)F]/D} \int_{x+L}^{x+2L} dy \, e^{[U(y)-yF]/D}
\]

\[
= \frac{1}{Z} e^{-[U(x)-(x+L)F]/D} \int_x^{x+L} dy \, e^{[U(z+L)-(z+L)F]/D}
\]

\[
= \frac{1}{Z} e^{-[U(x)-(x+L)F]/D} \int_x^{x+L} dz \, e^{[U(z)-Fz]/D}
\]

\[
= \frac{1}{Z} e^{-[U(x)-(x+L)F]/D} \int_x^{x+L} dz \, e^{[U(z)-(z+L)F]/D}
\]

\[
= p_\infty(x), \tag{1.125}
\]

A typical example is
\[ v_L(t) := \frac{1}{N_L(t)} \int_0^L dx \ j(t, x) = \frac{1}{N_L(t)} \int_0^L dx \ [F(t) - U'(x)] \ p(t, x) \]
\[ j_\infty = -[(\partial_x \Phi)p_\infty + D \partial_x p_\infty] \]

Inserting \( p_\infty(x) \) into Eq. (1.121) gives

\[
v_L = -\frac{1}{N_L} \int_0^L dx \ (\partial_x \Phi) \ p_\infty
\]
\[
= -\frac{1}{ZN_L} \int_0^L dx \ (\partial_x \Phi) \ e^{-\Phi(x)/D} \int_x^{x+L} dy \ e^{\Phi(y)/D}
\]
\[
= \frac{D}{ZN_L} \int_0^L dx \ [\partial_x e^{-\Phi(x)/D}] \int_x^{x+L} dy \ e^{\Phi(y)/D}. \quad (1.126)
\]
\[ v_L(t) := \frac{1}{N_L(t)} \int_0^L dx \ j(t, x) = \frac{1}{N_L(t)} \int_0^L dx \ [F(t) - U'(x)] \ p(t, x) \]

\[ \dot{j}_\infty = -[(\partial_x \Phi)p_{\infty} + D \partial_x p_{\infty}] \]

Inserting \( p_{\infty}(x) \) into Eq. (1.121) gives

\[
\begin{align*}
v_L &= -\frac{1}{N_L} \int_0^L dx \ (\partial_x \Phi) p_{\infty} \\
&= -\frac{1}{ZN_L} \int_0^L dx \ (\partial_x \Phi) e^{-\Phi(x)/D} \int_x^{x+L} dy \ e^{\Phi(y)/D} \\
&= \frac{D}{ZN_L} \int_0^L dx \ \left[ \partial_x e^{-\Phi(x)/D} \right] \int_x^{x+L} dy \ e^{\Phi(y)/D}.
\end{align*}
\] (1.126)

Integrating by parts, this can be simplified to

\[
\begin{align*}
v_L &= -\frac{D}{ZN_L} \int_0^L dx \ e^{-\Phi(x)/D} \partial_x \int_x^{x+L} dy \ e^{\Phi(y)/D} \\
&= -\frac{D}{ZN_L} \int_0^L dx \ e^{-\Phi(x)/D} \left[ e^{\Phi(x+L)/D} - e^{\Phi(x)/D} \right] \\
&= \frac{D}{ZN_L} \int_0^L dx \ \left\{1 - e^{[\Phi(x+L)-\Phi(x)]/D}\right\} \\
&= \frac{D}{ZN_L} \int_0^L dx \ \left\{1 - e^{-F[(x+L)-x]/D}\right\} \\
&= \frac{DL}{ZN_L} \left(1 - e^{-FL/D}\right), \quad (1.127)
\end{align*}
\]
\[ v_L(t) := \frac{1}{N_L(t)} \int_0^L dx \, j(t, x) = \frac{1}{N_L(t)} \int_0^L dx \, [F(t) - U'(x)] \, p(t, x) \]

\[ j_\infty = -[(\partial_x \Phi)p_\infty + D \partial_x p_\infty] \]

\[ v_L = \frac{DL}{ZN_L} \left( 1 - e^{-FL/D} \right) \]

where \( N_L \) can be expressed as

\[ N_L = \frac{1}{Z} \int_0^L dx \int_x^{x+L} dy \, e^{-[\Phi(x)-\Phi(y)]/D}. \quad (1.128) \]

We thus obtain the final result

\[ v_L = \frac{DL}{\int_0^L dx \int_x^{x+L} dy \, e^{-[\Phi(x)-\Phi(y)]/D}} \left( 1 - e^{-FL/D} \right), \quad (1.129) \]

which holds for arbitrary periodic potentials \( U(x) \). Note that there is no net-current at equilibrium \( F = 0 \).
Fig. 2.3. Typical example of an effective potential from (2.35) “tilted to the left”, i.e. \( F<0 \). Plotted is the example from (2.3) in dimensionless units (see Section A.4 in Appendix A) with \( L = V_0 = 1 \) and \( F = -1 \), i.e. \( V_{\text{eff}}(x) = \sin(2\pi x) + 0.25 \sin(4\pi x) + x \).

Fig. 2.4. Steady state current \( \langle \dot{x} \rangle \) from (2.37) versus force \( F \) for the tilted Smoluchowski–Feynman ratchet dynamics (2.5), (2.34) with the potential (2.3) in dimensionless units (see Section A.4 in Appendix A) with \( \eta = L = V_0 = k_B = 1 \) and \( T = 0.5 \). Note the broken point-symmetry.
1.6.2 Temperature ratchet

As we have seen in the preceding sections, the combination of noise and nonlinear dynamics can yield surprising transport effects. Another example is the so-called temperature-ratchet, which can be captured by the minimal SDE model

\[ dX(t) = [F - U'(X)] dt + \sqrt{2D(t)} dB(t), \quad (1.130a) \]

where \( D(t) = D(t + T) \) is now a time-dependent noise amplitude, such as for instance

\[ D(t) = \tilde{D} \{ 1 + A \text{ sign}[\sin(2\pi t/T)] \}, \quad (1.130b) \]

where \(|A| < 1\). Such a temporally varying noise strength can be realized by heating and cooling the ratchet system periodically. Transport can be quantified in terms of the combined spatio-temporal average

\[
\langle \dot{X} \rangle := \frac{1}{T} \int_{t}^{t+T} ds \int_{0}^{L} dx \, j(t, x) \\
= \frac{1}{T} \int_{t}^{t+T} ds \int_{0}^{L} dx \, [F - U'(x)] p(t, x). \quad (1.131)
\]

can be solved numerically
Time-dependent temperature

Fig. 2.5. Average particle current $\langle \dot{x} \rangle$ versus force $F$ for the temperature ratchet dynamics (2.3), (2.34), (2.47), (2.50) in dimensionless units (see Section A.4 in Appendix A). Parameter values are $\eta = L = T = k_B = 1$, $V_0 = 1/2\pi$, $\bar{T} = 0.5$, $A = 0.8$. The time- and ensemble-averaged current (2.53) has been obtained by numerically evolving the Fokker–Planck equation (2.52) until transients have died out.

Fig. 2.6. The basic working mechanism of the temperature ratchet (2.34), (2.47), (2.50). The figure illustrates how Brownian particles, initially concentrated at $x_0$ (lower panel), spread out when the temperature is switched to a very high value (upper panel). When the temperature jumps back to its initial low value, most particles get captured again in the basin of attraction of $x_0$, but also substantially in that of $x_0 + L$ (hatched area). A net current of particles to the right, i.e. $\langle \dot{x} \rangle > 0$ results. Note that practically the same mechanism is at work when the temperature is kept fixed and instead the potential is turned “on” and “off” (on–off ratchet, see Section 4.2).