Rotary Molecular Motors Driven by Transmembrane Ionic Currents

Charles S. Peskin
Courant Institute of Mathematical Sciences
New York University

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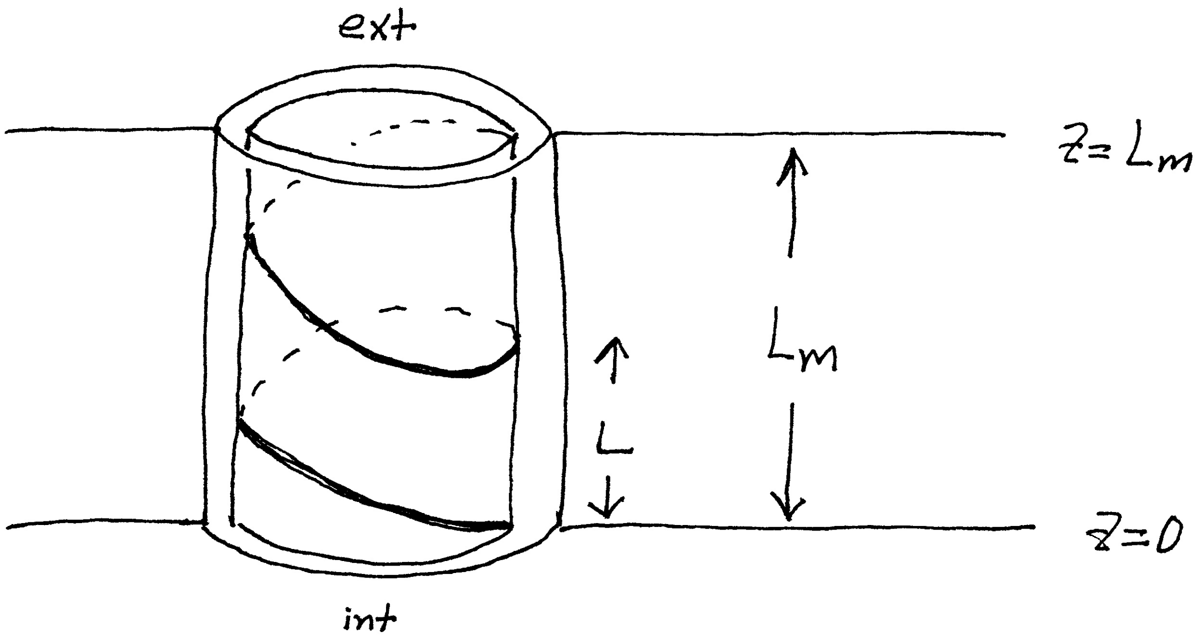

<u>rotor</u> : inner cylinder

<u>stator</u> : outer cylinder

L_m = membrane thickness

L = helical period

$L_m/L = n$, a positive integer

<u>Helical charge density on rotor:</u>

$$\sigma_{rotor} = -f\left(\theta + \omega t + 2\pi \frac{z}{L}\right)$$

$$f > 0, \quad f(\theta + 2\pi) = f(\theta)$$

<u>Sign convention</u> (viewed from above)

θ increases <u>counterclockwise</u> (as usual)

$\omega > 0$ denotes <u>clockwise</u> rotation

helix winds <u>clockwise</u> as z increases

Equations for charge density and current density of ions on stator, and for the electrostatic potential ϕ

Charge conservation:

(1) $$\frac{\partial \sigma}{\partial t} + \frac{\partial J}{\partial z} = 0$$

Longitudinal diffusion & drift:

(2) $$J = -D\left(\frac{\partial \sigma}{\partial z} + \frac{\delta}{kT}\frac{\partial \phi}{\partial z}\sigma\right)$$

Electroneutrality:

(3) $$\sigma = -\sigma_{rotor} = f\left(\theta + \omega t + 2\pi \frac{z}{L}\right)$$

σ = charge/area on stator

J = longitudinal current/length on stator (positive upwards)

ϕ = electrostatic potential

q = charge on each ion ($q > 0$)

k = Boltzmann's constant

T = absolute temperature

D = diffusion coefficient of ions on stator

$$\frac{D}{kT} q \left(-\frac{\partial \phi}{\partial z} \right) = \text{drift velocity of ions on stator}$$

$\frac{kT}{q} = 25 \, mV$ (if each ion carries one elementary charge)

Boundary conditions:

$$\sigma_{z=0^+} = K q C_{int} \exp\left(-\frac{q(\phi_{z=0^+} - \phi_{int})}{kT}\right) \tag{4}$$

$$\sigma_{z=L_m^-} = K q C_{ext} \exp\left(-\frac{q(\phi_{z=L_m^-} - \phi_{ext})}{kT}\right) \tag{5}$$

Since L_m/L is an integer, where L is the helical period,

$$\sigma_{z=0^+} = \sigma_{z=L_m^-} = f(\theta + \omega t) \tag{6}$$

let

$$\Phi = \phi_{z=L_m^-} - \phi_{z=0^+} \tag{7}$$

$$= \phi_{ext} - \phi_{int} + \frac{kT}{q} \log \frac{C_{ext}}{C_{int}}$$

independent of θ and t

<u>Arithmetic and Harmonic mean of f</u> $(f>0)$

(8) $$f_A = \frac{1}{2\pi}\int_0^{2\pi} f(\theta)\,d\theta$$

(9) $$f_H = \left(\frac{1}{2\pi}\int_0^{2\pi} \frac{d\theta}{f(\theta)}\right)^{-1}$$

Then

(10) $$f_A \geq f_H$$

with equality only if f is constant.

<u>Proof</u>: Apply Schwarz inequality to

(11) $$1 = \frac{1}{2\pi}\int_0^{2\pi} f^{1/2}(\theta)\, f^{-1/2}(\theta)\,d\theta$$

Evaluation of J:

From (1) & (3),

(12) $$\frac{\partial J}{\partial z} = -\omega f'\left(\theta + \omega t + \frac{2\pi}{L} z\right)$$

(13) $$J = -\frac{\omega L}{2\pi} f\left(\theta + \omega t + \frac{2\pi}{L} z\right) + J_0$$

where J_0 may depend on (θ, t) but not z. To find J_0, divide by σ $(= f)$ in (2) and integrate dz over $(0, L_m)$. Note that

(14) $$\int_0^{L_m} \frac{1}{\sigma} \frac{\partial \sigma}{\partial z} dz = 0$$

because of periodicity

In this way,

(15) $$J_0 = \left(\frac{\omega L}{2\pi} - \frac{D}{L_m}\frac{q\Phi}{kT}\right) f_H$$

and then

(16) $$J = -\frac{\omega L}{2\pi}\left(f - f_H\right) - \frac{D}{L_m}\frac{q\Phi}{kT} f_H$$

The total current I, positive <u>downward</u> is then given by

(17) $$I = -2\pi r J_A$$

$$= \omega r L\left(f_A - f_H\right) + 2\pi r \frac{D}{L_m}\frac{q\Phi}{kT} f_H$$

$$= rL\left(\omega\left(f_A - f_H\right) + q\frac{D}{kT}\frac{2\pi}{L L_m} f_H \Phi\right)$$

where r = radius of stator
= radius of rotor (tight fit !)

Evaluation of torque

Let τ = externally applied torque to the rotor (positive clockwise, like ω). This must be balanced by internal torque on the rotor, positive counterclockwise, produced by the electric field $-\nabla\phi$ acting on the charge density $\sigma_{rotor} = -f$. Therefore,

(18) $$\tau = \int_0^{L_m}\int_0^{2\pi} r\left(-\frac{1}{r}\frac{\partial\phi}{\partial\theta}\right)\left(-f\right) r\,d\theta\,dz$$

We can evaluate this integral without explicitly knowing ϕ by the following steps (IBP = integrate by parts):

(i) IBP to move $\frac{\partial}{\partial \theta}$ from ϕ to f

(ii) Use form of f to change $\frac{\partial}{\partial \theta}$ to $\frac{\partial}{\partial z}$

(iii) IBP to move $\frac{\partial}{\partial z}$ from f back to ϕ.

(iv) Use equation (2) and note that $\int_0^{L_m} \frac{\partial \sigma}{\partial z} dz = 0$.

The details are as follows:

(19) $$\tau = -r\int_0^{L_m}\int_0^{2\pi} \phi \frac{\partial f}{\partial \theta}\, d\theta\, dz$$

$$= -\frac{rL}{2\pi}\int_0^{2\pi}\int_0^{L_m} \phi \frac{\partial f}{\partial z}\, dz\, d\theta$$

$$= -\frac{rL}{2\pi}\int_0^{2\pi} \Phi f\, d\theta + \frac{rL}{2\pi}\int_0^{2\pi}\int_0^{L_m} \frac{\partial \phi}{\partial z} f\, dz\, d\theta$$

$$= -rL\Phi f_A - \frac{rL}{2\pi D}\frac{kT}{\xi}\int_0^{L_m}\int_0^{2\pi} J\, d\theta\, dz$$

$$= -rL\Phi f_A + \frac{L L_m}{2\pi D}\frac{kT}{\xi} I$$

We now have two linear equations, (17) & (19) that relate the four variables

$$\omega, \; I, \; \tau, \; \Phi$$

and we can solve for (ω, I) in terms of (τ, Φ):

$$(20) \qquad \begin{pmatrix} \omega \\ I \end{pmatrix} = q \frac{D}{kT} \frac{2\pi}{LL_m} \begin{pmatrix} \frac{1}{rL(f_A - f_H)} & 1 \\ 1 & rLf_A \end{pmatrix} \begin{pmatrix} \tau \\ \Phi \end{pmatrix}$$

Note that the matrix in (20) is symmetric, and it is also positive definite since its trace and determinant are both positive (and for a 2×2 matrix this implies positive definiteness).

In the language of irreversible thermodynamics,

τ, Φ are forces

ω, I are the <u>corresponding</u> fluxes

The correspondance is that

$\tau\omega$ = power applied by τ

ΦI = power applied by Φ

It is a general principle, discovered by Onsager, that in a near-equilibrium system fluxes are linearly related to forces by a positive-definite symmetric matrix. We have an instance of that here, without necessarily being near equilibrium.

Two special cases:

(i) Free rotation ($\tau = 0$)

(21) $$\omega_{free} = q \frac{D}{kT} \frac{2\pi}{L L_m} \Phi$$

(22) $$I_{free} = q \frac{D}{kT} \frac{2\pi r f_A}{L_m} \Phi$$

(ii) Stall ($\omega = 0$)

(23) $$\tau_{stall} = -rL(f_A - f_H)\Phi$$

(24) $$I_{stall} = q \frac{D}{kT} \frac{2\pi r f_H}{L_m} \Phi$$

Some remarks:

(i) In the free-rotation case

$$L \frac{\omega_{free}}{2\pi} = \frac{g}{\gamma} \frac{D}{kT} \frac{\Phi}{Lm} \tag{25}$$

that is,

velocity of helical wave = drift velocity of ions in the stator

so the ions are surfing the helical wave!

(ii) $$\frac{I_{stall}}{I_{free}} = \frac{f_H}{f_A} < 1 \tag{26}$$

and this is very different from an ordinary electric motor, in which stalling the motor produces a short-circuit condition and a large, dangerous current.

(iii) The helical wavelength L has opposite effects on ω_{free} and τ_{stall}.

To make the motor fast, L should be small, i.e., the helix should be tightly wound, but such a motor can bear very little load.

To make τ_{stall} as large as possible, the best choice of L is L_m (which is the largest possible choice to which our theory applies, since L_m/L is supposed to be a positive integer).

Design of the motor to operate at a given $\omega > 0$, and given $\tau = -\tau_{load}$ with $\tau_{load} > 0$

From (20)

(27) $$\Phi = \frac{\omega}{A} + \frac{\tau_{load}}{B(1-\alpha)}$$

(28) $$I = B\omega + A\alpha\,\tau_{load}$$

where

(29) $$A = \gamma \frac{D}{kT} \frac{2\pi}{L L_m}$$

(30) $$B = r L f_A$$

(31) $$\alpha = \frac{f_H}{f_A} \in [0, 1]$$

The power that must be supplied by the ionic current is given by

(32) $$P = \Phi I = \frac{B}{A}\omega^2 + \left(\alpha + \frac{1}{1-\alpha}\right)\omega \tau_{load} + \frac{A}{B}\frac{\alpha}{1-\alpha}\tau_{load}^2$$

Note that $P > \omega \tau_{load}$, as it must be since $\omega\tau_{load}$ is the power delivered to the load.

For fixed α, we can minimize P as a function of B/A by setting

(33) $$\frac{B}{A} = \sqrt{\frac{\alpha}{1-\alpha}}\ \frac{\tau_{load}}{\omega}$$

This gives an explicit formula for the optimal helical wavelength

$$(34) \qquad L_{opt}^{2} = 4\pi^2 \frac{q}{2\pi r L_m f_A} \frac{D}{kT} \frac{\tau_{load}}{\omega} \sqrt{\frac{\alpha}{1-\alpha}}$$

Strictly speaking, we should have done discrete optimization over those L for which L_m/L is a positive integer, but we ignore that restriction here.

If we evaluate P with B/A given by (33), we get

(35) $$P_{opt} = \left(\sqrt{\alpha} + \sqrt{\frac{1}{1-\alpha}}\right)^2 \omega \tau_{load}$$

and this shows that the maximum possible efficiency of the motor is determined by $\alpha = f_H/f_A$ and is given by

(36) $$E_{max} = \frac{\omega \tau_{load}}{P_{opt}} = \frac{1}{\left(\sqrt{\alpha} + \sqrt{\frac{1}{1-\alpha}}\right)^2}$$

This decreases from 1 to 0 as α goes from 0 to 1.

Fluctuations

Let the motor be rigidly connected to a load with rotational drag coefficient γ, that is

(37) $$-\tau = \tau_{load} = \gamma\omega$$

Then, from (27-32),

(38) $$\Phi = \omega\left(\frac{1}{A} + \gamma\frac{1}{B(1-\alpha)}\right)$$

(39) $$I = \omega\left(B + \gamma A\alpha\right)$$

(40) $$P = \omega^2\left(\frac{B}{A} + \gamma\left(\alpha + \frac{1}{1-\alpha}\right) + \gamma^2\frac{A}{B}\frac{\alpha}{1-\alpha}\right)$$

Let ω^* be the solution of (38):

$$(41) \qquad \omega^* = \frac{\Phi}{\frac{1}{A} + \gamma \frac{1}{B(1-\alpha)}}$$

and let

$$(42) \qquad \gamma^* = \frac{B}{A} + \gamma\left(\alpha + \frac{1}{1-\alpha}\right) + \gamma^2 \frac{A}{B} \frac{\alpha}{1-\alpha}.$$

so that (40) becomes

$$(43) \qquad P = \omega^2 \gamma^*$$

Thus ω^* is the macroscopic angular velocity (clockwise positive) and γ^* is the effective rotational drag coefficient of the motor connected to the load.

Thus, if we consider an ensemble of such systems each at temperature T, the probability density function $\rho(\theta, t)$ satisfies the constant-coefficient drift-diffusion equation

$$(44) \qquad \frac{\partial \rho}{\partial t} - \omega^* \frac{\partial \rho}{\partial \theta} = \frac{kT}{\gamma^*} \frac{\partial^2 \rho}{\partial \theta^2}$$

and this diffusion equation governs the fluctuations in θ. (The minus sign on the left-hand side is because ω^* is positive for clockwise rotation, but θ increases counterclockwise.)