Autonomous Brownian Motors

AI

1 The Büttiker-Landauer model [1, 2]

We consider the Langevin equation for the variable x driven by multiplicative noise,

$$\dot{x} = h(x) + g(x)\xi(t), \tag{1}$$

with $\xi(t)$ a Gaussian white noise, $\langle \xi(t)\xi(t')\rangle = 2\delta(t-t')$. The force is derived by some L-periodic potential $h(x) = -\partial_x V(x)$. For a constant $g = \sqrt{T}$, the Langevin equation (1) describes a Brownian particle subject to the force $h(x)$ that, starting from an arbitrary initial condition, reaches an equilibrium thermal state in the long time limit. However, for a position dependent temperature profile $g(x) = \sqrt{T(x)}$, the system will be in an out–of–equilibrium state. In the following we assume that $T(x)$ is also L-periodic. Using the Stratonovich interpretation the Fokker-Planck equation has the form $dP/dt = -dJ/dx$, where the probability current is given by

$$J(x) = (h(x) - g(x)g(x)')P(x) - g^2(x)P'(x). \tag{2}$$

The steady state solution reads

$$P(x) = \frac{\mathrm{e}^{-U(x)}}{g(x)}\left[c_1 - c_2 I(x)\right], \tag{3}$$

where we have introduced the effective potential

$$U(x) = -\int_0^x \mathrm{d}y\, \frac{h(y)}{g^2(y)}, \tag{4}$$

and defined

$$I(x) = \int_0^x \mathrm{d}y\, \frac{\mathrm{e}^{U(y)}}{g(y)}. \tag{5}$$

Imposing the periodicity condition on the steady state solution (3), i.e., $P(0) = P(L)$, and noticing that $g(x)$ is periodic, $g(0) = g(L)$, and that $U(0) = I(0) = 0$, we obtain

$$c_1 = \mathrm{e}^{-U(L)} \left[c_1 - c_2 I(L) \right] \tag{6}$$

which can be solved for c_1 only if $U(L) \neq 0$, see discussion below.

The L-periodic stationary solution of the FP equation reads

$$\begin{aligned} P(x) &= c_2 \frac{\mathrm{e}^{-U(x)}}{g(x)} \left(\frac{I(L)}{1 - \mathrm{e}^{U(L)}} - I(x) \right) \\ &= c_2 \frac{\mathrm{e}^{-U(x)}}{(1 - \mathrm{e}^{\bar{f}L}) g(x)} \int_x^{x+L} \frac{\mathrm{e}^{U(y)}}{g(y)}\, dy, \end{aligned} \tag{7}$$

with $\bar{f} = U(L)/L = [U(x+L) - U(x)]/L$.

The normalization condition $\int_0^L dx P(x) = 1$ then yields the constant steady-state current

$$c_2 = \bar{J} = (1 - \mathrm{e}^{\bar{f}L}) \left[\int_0^L dx \frac{\mathrm{e}^{-U(x)}}{g(x)} \int_x^{x+L} dy \frac{\mathrm{e}^{U(y)}}{g(y)} \right]^{-1}, \tag{8}$$

and thus the non zero propagation velocity $\bar{v} = L\bar{J}$. Here the quantity $\bar{f} = [U(x+L) - U(x)]/L$ is a generalized thermodynamic force and quantifies the breaking of the right-left symmetry. It is non-zero if the function $U(x)$ is non-periodic. The quantity $\bar{f}L$ is the entropy change in the bath upon completing a cycle $x = 0 \to L$,

Taking, for example, $V(x) = V_0 \sin(x)$, $T(x) = g^2(x) = T_0 + \Delta T \sin(x + \phi)$, one finds

$$U(L) = 2\pi \frac{V_0}{\Delta T} \left(1 - \frac{T_0}{\sqrt{T_0^2 - \Delta T^2}} \right) \sin(\phi) \tag{9}$$

for $\Delta T \neq 0$.

A few plots of the steady–state current for the potential $V(x) = V_0 \sin(x)$ and the temperature profile $T(x) = T_0 + \Delta T \sin(x + \phi)$ are shown in fig. 1. Inspection of the figure indicates that the current is zero when $\phi = 0, \pi$ (spatial symmetry) and maximal for $\phi = \pi/2$ which correspond to the most asymmetrical configuration.

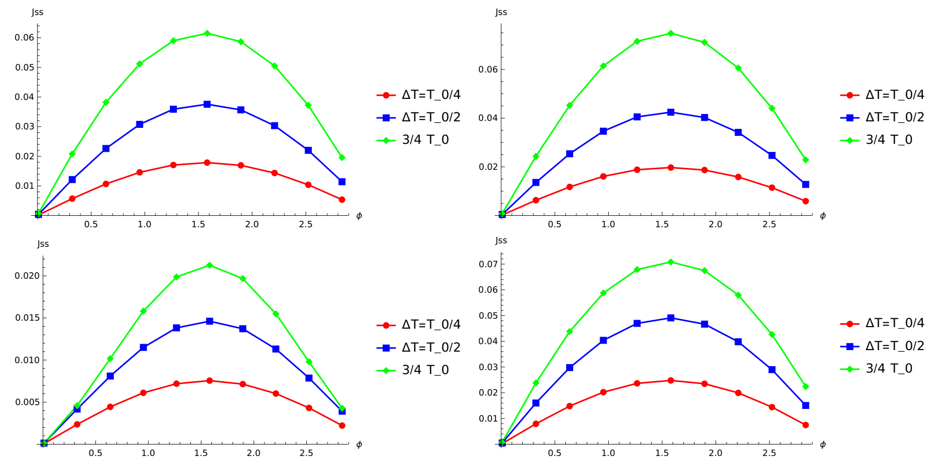

Figure 1: Steady state current for the BL model, eq. (8), with $V(x) = V_0 \sin(x)$ and $T(x) = T_0 + \Delta T \sin(x + \phi)$ for different values of the parameters V_0, T_0, and ΔT. Top left, $V_0 = 1$, $T_0 = 2$, top right $V_0 = 1$, $T_0 = 4$, bottom left $V_0 = 2$, $T_0 = 1$, bottom right $V_0 = 2$, $T_0 = 2$.

2 Two particles at different temperatures

The model consists of two overdamped coupled degrees of freedom moving in periodic potentials and driven by two heat reservoirs maintained at different temperatures T_1 and T_2. Denoting the degrees of freedom by x_1 and x_2, the model is characterized by the potential

$$V(x_1, x_2) = V_1(x_1) + V_2(x_2) + kv(x_1 - x_2), \tag{10}$$

where V_i are periodic potentials with period L, and $kv(x_1 - x_2)$ a periodic interaction potential, with interaction strength k, (ex. $v(z) = -\cos(z)$). Setting the friction constant $\Gamma = 1$ and denoting the forces by $F_i = -dV_i/dx_i$ the overdamped coupled Langevin equations have the form (a dot denoting a time derivative, a prime denoting a space derivative)

$$\dot{x}_1 = F_1(x_1) - kv'(x_1 - x_2) + \eta_1(t), \tag{11}$$
$$\dot{x}_2 = F_2(x_2) - kv'(x_2 - x_1) + \eta_2(t); \tag{12}$$

here the white Gaussian noises η_1 and η_2, characterizing the heat reservoirs at temperatures T_1 and T_2, are correlated according to $\langle \eta_i(t)\eta_j(t')\rangle = 2T_i\delta_{ij}\delta(t - t')$.

We introduce the two variables $x = (x_1 + x_2)/2$ and $y = (x_1 - x_2)/2$, and notice that for large coupling k the variable y is suppressed allowing the expansions

$$F_1(x_1) \simeq F_1(x) + F_1'(x)y, \quad F_2(x_2) \simeq F_2(x) + F_2'(x)y. \tag{13}$$

By insertion we obtain

$$\dot{x} = \frac{1}{2}\left[F_1(x) + F_2(x)\right] + \frac{y}{2}\left[F_1'(x) - F_2'(x)\right] + \frac{1}{2}(\eta_1 + \eta_2), \tag{14}$$

$$\dot{y} = \frac{1}{2}\left[F_1(x) - F_2(x)\right] + \frac{y}{2}\left[F_1'(x) + F_2'(x)\right] - 2ky + \frac{1}{2}(\eta_1 - \eta_2), \tag{15}$$

where we have used $v'(y) \simeq y$. Imposing $\dot{y} = 0$, from eq. (15) one finds

$$y = \frac{F_1(x) - F_2(x) + \eta_1 - \eta_2}{4k - (F_1'(x) + F_2'(x))} \tag{16}$$

and by substituting eq. (16) in eq. (14) a single Langevin equation for the center of mass coordinate,

$$\begin{aligned} \dot{x} &= (F_1(x) + \eta_1(t))s_1(x) + (F_2(x) + \eta_2(t))s_2(x) \\ &= h(x) + g(x)\xi(t), \end{aligned} \tag{17}$$

where

$$h(x) = F_1(x)s_1(x) + F_2(x)s_2(x), \tag{18}$$

$$s_1(x) = \frac{2k - F_2'(x)}{4k - (F_1'(x) + F_2'(x))}, \tag{19}$$

$$s_2(x) = \frac{2k - F_1'(x)}{4k - (F_1'(x) + F_2'(x))}, \tag{20}$$

and

$$g(x) = \sqrt{T_1 s_1^2(x) + T_2 s_2^2(x)}. \tag{21}$$

with $\xi(t)$ a Gaussian white noise, $\langle \xi(t)\xi(t') \rangle = 2\delta(t - t')$. We are thus back to the case discussed in the previous section.

Taking, for example, $V_1(x) = V_0 \sin(x)$ and $V_2(x) = V_0 \sin(x+\phi)$ one can calculate $U(L=2\pi)$ in two limiting cases:

i) for $k \gg V_0$, T one finds

$$U(L) = 2\pi \frac{(T_2 - T_1)}{(T_1+T_2)^2} \frac{V_0^2}{k} \sin\phi + O(1/k^2). \tag{22}$$

ii) up to first order in ϕ one finds

$$U(L) = 16k\pi\phi \frac{(T_2 - T_1)}{(T_1+T_2)^2} + O(\phi^3). \tag{23}$$

In the general case the current and thus the velocity, as given by

$$\bar{v} = \frac{1}{2}\langle \dot{x}_1 + \dot{x}_2 \rangle = -\frac{1}{2}\langle V_1'(x_1) + V_2'(x_2) \rangle \tag{24}$$

can be obtained numerically by, e.g., solving the FP equation.

In fig. 2 a few results for the current are shown for different choices of the parameters, and a potential given by

$$V(x_1, x_2) = \cos(nx_1) + \cos(nx_2 + \phi) - k\cos[n(x_1 - x_2)]. \tag{25}$$

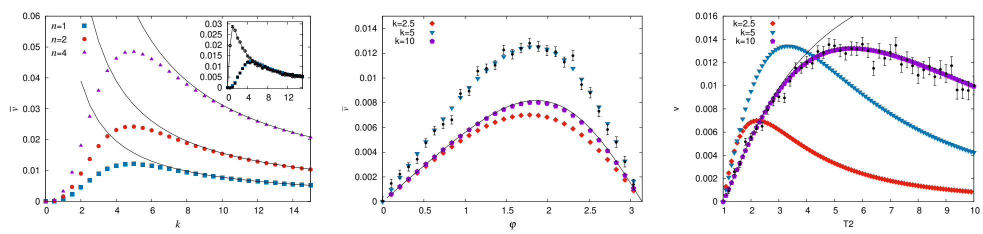

Figure 2: Center-of-mass velocity $\bar{v}$ for the two-particle system with potential (25). Left panel: $\bar{v}$ as a function of the interaction strength k for different values of n, with $\phi = \pi/2$, $T_1 = 1$, $T_2 = 2.5$. Center: $\bar{v}$ as a function of the phase ϕ for different values of k, with $n = 1$, $T_1 = 1$, $T_2 = 2.5$. Right: $\bar{v}$ as a function of ΔT, with $T_1 = 1$, $T_2 = T_1 + \Delta T$, $n = 1$, $\phi = \pi/2$.

3 Two rotors

A system made up of two rotors in contact with two heat baths also behave as a rectifier.

Let us consider the two–rotor model with interaction energy

$$U(n_1, n_2) = -k\cos[(n_1 - n_2)\alpha + \phi], \tag{26}$$

with $\alpha = 2\pi/N_s$, $n_i = 0, 1 \ldots N_s$. We see that when $\phi = l\pi/N_s$, with l an integer, the energy is symmetric with respect to particle swap combined with a rotation of a single spin, i.e. there exist an integer δ such that

$$U(-n_1, -n_2) = U(n_1 + \delta, n_2), \tag{27}$$

for all n_1 and n_2. This symmetry is broken if $\phi \neq l\pi/N_s$

We require that the transition rates obey the local detailed balance condition (LDBC)

$$\frac{W_1(n_1', n_2 \leftarrow n_1, n_2)}{W_1(n_1, n2 \leftarrow n_1', n_2)} = \mathrm{e}^{-\beta_1[U(n_1', n_2) - U(n_1, n_2)]}, \tag{28}$$

$$\frac{W_2(n_1, n_2' \leftarrow n_1, n_2)}{W_2(n_1, n2 \leftarrow n_1, n_2')} = \mathrm{e}^{-\beta_2[U(n_1, n_2') - U(n_1, n_2)]}. \tag{29}$$

There are several choices for the transition rates that satisfy the LDBC, and here we use the symmetric rates

$$W_i(s' \leftarrow s) = \omega_0 \mathrm{e}^{-\frac{\beta_i}{2}[U(s') - U(s)]}, \tag{30}$$

with this choice the steady–state PDF reads

$$P^{ss}(n_1, n_2) = \exp\left[-\frac{\beta_1 + \beta_2}{2} U(n_1, n_2)\right]/\mathcal{N}, \tag{31}$$

where $\mathcal{N}$ is a normalization constant. This result holds only for the specific choice of the rates (29).

Once $P^{ss}(n_1, n_2)$ one can obtain the steady state currents, for example J_2^{ss} reads

$$J_2^{ss} = \sum_{n1=0}^{N_s-1} W_1(n_1, n_2 \leftarrow n_1, n_2{-}1) P^{ss}(n_1, n_2{-}1) - W_1(n_1, n_2 \leftarrow n_1, n_2{+}1) P^{ss}(n_1, n_2{+}1), \tag{32}$$

and is independent of n_2. The analogous expression gives J_1^{ss}.

For $N_s = 3$ and in the limit of small ϕ one finds

$$J_1^{ss} = J_2^{ss} = \omega_0 \phi k \frac{\beta_1(1 - e^{3\beta_2 k/4}) - \beta_2(1 - e^{3\beta_1 k/4})}{2\sqrt{3}(2 + e^{3(\beta_1+\beta_2)k/4})} \tag{33}$$

For $N_s = 3$ and the specific choice $\phi = \alpha/4 = \pi/6$ one finds

$$J_1^{ss} = J_2^{ss} = \omega_0 \frac{(\gamma_1 - 1)(\gamma_2 - 1)(\gamma_1 - \gamma_2)}{3\left[1 + \gamma_1\gamma_2 + (\gamma_1\gamma_2)^2\right]}, \tag{34}$$

with $\gamma_i = e^{\beta_i \frac{k}{2} \cos(\pi/6)}$.

The heat currents are given by

$$\left\langle \dot{Q}_1 \right\rangle = \sum_{n_1, n_1'=0}^{N_s-1} P^{ss}(n_1, n_2) W_1(n_1', n_2 \leftarrow n_1, n_2)(U(n_1', n_2) - U(n_1, n_2))$$

$$\left\langle \dot{Q}_2 \right\rangle = \sum_{n_2, n_2'=0}^{N_s-1} P^{ss}(n_1, n_2) W_2(n_1, n_2' \leftarrow n_1, n_2)(U(n_1, n_2') - U(n_1, n_2))$$

One can evaluate explicitly the heath current for $N_s = 3$ and $\phi = \alpha/4 = \pi/6$

$$\left\langle \dot{Q}_1 \right\rangle = \omega_0 k \frac{\sqrt{3}}{2} \frac{(\gamma_2 - \gamma_1)(1 + 2(\gamma_1 + \gamma_2) + \gamma_1\gamma_2)}{1 + \gamma_1\gamma_2 + (\gamma_1\gamma_2)^2} = -\left\langle \dot{Q}_2 \right\rangle. \tag{35}$$

One can add a counteracting force (torque here) to one of the particles, e.g. f_1, the potential thus becomes

$$\mathcal{U}(n_1, n_2, f_1) = U(n_1, n_2) - f_1 n_1. \tag{36}$$

In the regime where $f_1 < 0$ is not too large the system behaves as a machine able to convert heat current $\left\langle \dot{Q}_H \right\rangle$ into mechanical work with rate $-f_1 \bar{v}_1$. One can then solve numerically the master equation and evaluate the power $P_{out} = -f_1 \bar{v}_1$ and the efficiency

$$\eta = \frac{-f_1 \bar{v}_1}{\left\langle \dot{Q}_H \right\rangle}. \tag{37}$$

Results obtained by numerical solution of the master equation with $N_s = 3$ are shown in fig. (3).

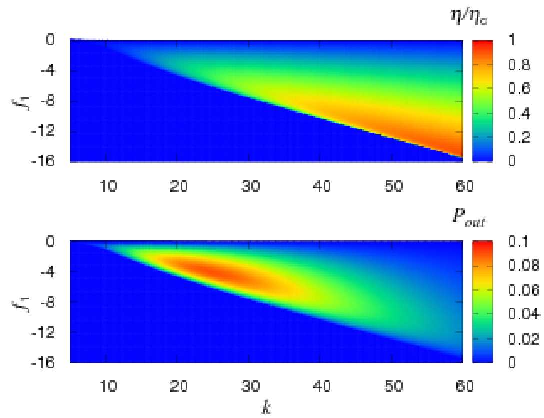

Figure 3: Power and efficiency of the model (36) as functions of k and f_1

References

[1] Rolf Landauer. Motion out of noisy states. *Journal of Statistical Physics*, 53(1):233–248, 1988.

[2] Ronald Benjamin and Ryoichi Kawai. Inertial effects in büttiker-landauer motor and refrigerator at the overdamped limit. *Phys. Rev. E*, 77:051132, May 2008.