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Non-equilibrium directed diffusion and inherently irreversible heat engines

I M Sokolov† and A Blumen

Theoretische Polymerphysik, Universität Freiburg, Rheinstraße 12, D-79104 Freiburg i. Br., Germany

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Abstract. We consider models which are symmetric under time-reversal and which produce net currents under parametrical, dichotomous, thermal excitation. The simplest is based on a three-level system, which is the basic unit of a 'minimal' thermally driven ratchet. We analyse the system's behaviour under periodic, dichotomous temperature changes and calculate the current, work and efficiency of the engine as functions of the upper and lower temperatures and of the modulation period. The system's behaviour differs greatly from a quasistatically working heat engine (such as based on a Carnot cycle). We discuss how this behaviour arises due to the inherently irreversible nature of the underlying process.

1. Introduction

There are at least four important reasons for considering a kinetic three-level system under dichotomous parametrical excitation.

First, the system is related to a class of thermal ratchets [1–8], which are under extensive investigation as models for molecular motors, possibly leading to the understanding of the principles of muscle action [9]. Corresponding effects in artificial systems were observed experimentally [10, 11], and the debate concerning applications to kinesin is still open [12]. The system which we present is a discrete, minimal model for a molecular ratchet; it shows asymmetric transitions under external modulation. Secondly, the discrete system considered belongs to a class which has recently won attention by showing coherent stochastic resonance [13–15]. Here we are interested in a related, but somewhat different effect, namely in the appearance of strong coupling between the high-frequency modes (here: temperature cycles) and zero-frequency modes (here: overall current) which emerge in our linear model due to parametrical excitation. Thirdly, the system can be viewed thermodynamically as a machine which works between two heat reservoirs, and offers a paradigmal description of inherent irreversibility. By this we mean that it is fundamentally different from usual heat engines: these work as (non-ideal approximations to) reversible engines, which undergo slow (quasistatic) changes [16]; the system we are interested in works best when the temperature changes are sudden, and the duration of the cycles is short. Fourthly, we are confronted here with non-equilibrium directed diffusion, an effect which offers the possibility of experimental checks. Thus, the response of cellular molecular motors to periodic temperature changes may provide clues to the relevance of ratchets in biological systems.

† Also at: P N Lebedev Physical Institute of the Academy of Sciences of Russia, Leninsky Prospekt 53, Moscow 117924, Russia.

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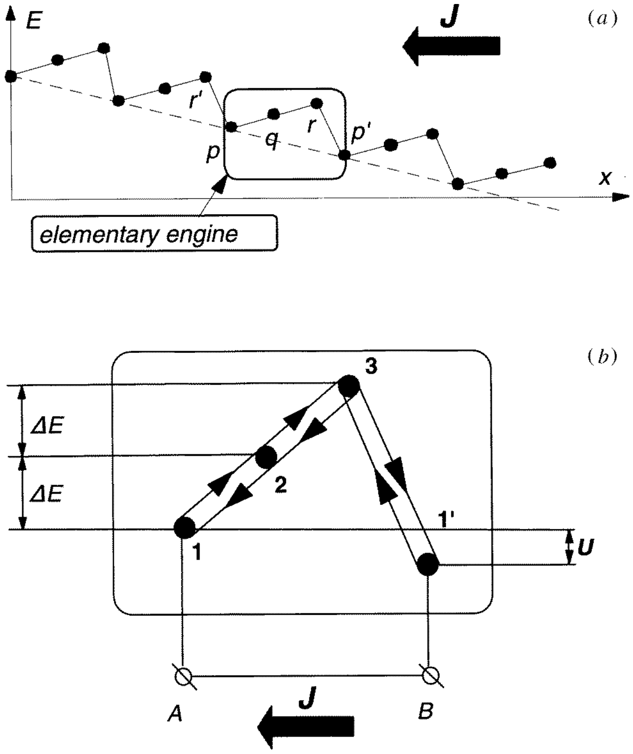

Figure 1. (*a*) The structure of the array used and (*b*) the construction of the elementary engine. The arrow shows the direction of short-circuit current.

2. The model

Here we deal with a discrete model formulated within the master-equation description for continuous-time random walks of particles on a one-dimensional lattice. This parallels the approaches considered in [14, 15], see figure 1:

$$\frac{\partial}{\partial t} p_n(t) = w_{n-1,n}(t) p_{n-1}(t) + w_{n+1,n}(t) p_{n+1}(t) - (w_{n,n-1} + w_{n,n+1}) p_n(t). \tag{1}$$

Here $p_n(t)$ is the probability density of finding a particle at the site n at time t, and w_{ij} are the transition rates between neighbouring sites i and j. Under an appropriate choice of these (time-dependent) transition rates (which then mirror the site energies E_i of a given potential) equation (1) is a discrete version of a thermal ratchet. We are in a discrete picture, which differs from the usual continuous description [1–8] based on the Langevin (or, equivalently on the corresponding Fokker–Planck) equation.

We confine ourselves to a stationary and spatially homogeneous situation in which the populations $p_n(t)$ of corresponding sites are periodic; this is depicted in figure 1(*a*) using $k = 3$ as a period. The overall system consists of an array of elements, figure 1(*b*), which are switched in succession. In the discussion we can focus on the determination of the properties of single elements. It is of interest to know in which range of parameters the system produces on average a directed current and thus work; for this we also calculate the efficiency of the elements. The work consists of maintaining an uphill current against the overlaid constant potential gradient (see figure 1). This gradient is the difference (in figure 1(a) denoted by U) between the potential energies of the sites (say 1) of successive elements.

We take the forward rates to equal $w_{ij} = 1$ (provided $E_j < E_i$); the backward rates are $w_{ji} = \exp(-\frac{E_i - E_j}{k_B T})$. This thermally activated form ensures that in equilibrium detailed balance is obeyed. We suppose (as is physically reasonable) that under temperature changes the local thermal equilibration is much faster than the equilibration of the concentrations. Such temperature changes lead to the breakdown of detailed balance, which mechanism drives the engine. As may be inferred on physical grounds and as we proceed to discuss, we find that the smallest engine which produces an overall current under thermal modulation is based on a three-level system. A two-level system, on the other hand, does not produce any net current; this can also be shown analytically, using the formalism we are going to present.

We turn now to the description of the three-level element, see figure 1(b). We fix the energy at site 1 as $E = 0$ and let sites 2 and 3 have energies ΔE and $2\Delta E$ respectively; the energy of particles on site 1′ (the first site of the next element) is taken to be $-U$. We denote the corresponding backward rates by x and y:

$$\begin{aligned} y &= w_{12} = w_{23} = \exp\left(-\frac{\Delta E}{k_B T}\right) \\ x &= w_{1'3} = \exp\left(-\frac{2\Delta E + U}{k_B T}\right). \end{aligned} \tag{2}$$

For ease of notation we set $k_B = 1$ and take $\Delta E = 1$ so that both U and T are measured in units of ΔE. Now the backward rates depend on time through the time-dependence of ΔE or of T. Here we let T depend on time, a procedure which allows us to make a connection to thermodynamics and to compare the (very unusual) properties of our highly non-equilibrium heat engine with those of standard, equilibrium engines. Previous works concentrated on the fascinating property of ratchets to produce an average net current from noise. Our elementary engine has the same property and we consider here a periodic, parametrical thermal modulation; this parallels, to some extent, the periodically rocked model of [5]. Thus we bring the engine alternatingly for times, τ, in contact with a warm (temperature T_1) and with a cold (temperature T_2) heat reservoir. Thus:

$$T(t) = \begin{cases} T_1 & 2n\tau < t < (2n+1)\tau \\ T_2 & (2n+1)\tau < t < 2(n+1)\tau \end{cases} \tag{3}$$

and the period is 2τ.

Let us consider the equations obeyed by the three-level element. The momentary state of the engine is characterized by the occupation numbers of its sites 1, 2 and 3 which we denote by p, q and r respectively. These occupation numbers are governed by the following system of ordinary differential equations (ODE):

$$\begin{aligned} \dot{p} &= -(x+y)p + q + r' \\ \dot{q} &= yp - (1+y)q + r \\ \dot{r} &= xp' + yq - 2r \end{aligned} \tag{4}$$

where r' is the occupation number of site 3 of the element at the left and p' is the occupation number of site 1 of the element at the right. In a stationary, spatially homogeneous situation one has $r' = r$ and $p' = p$. In this case also $\frac{\mathrm{d}}{\mathrm{d}t}(p+q+r) = 0$ holds (conservation law), i.e. $p + q + r =$ constant. Taking the number of particles per engine to be unity

$$p + q + r = 1 \tag{5}$$

reduces equation (3) to the following closed system of two, coupled ODE

$$\begin{aligned}\dot{p} &= 1 - (1 + x + y)p \\ \dot{q} &= 1 + (y - 1)p - (2 + y)q.\end{aligned} \tag{6}$$

Here one should remember that the transition rates x and y depend on time through temperature. Note that in general an element consisting of k levels obeys a set of $k - 1$ coupled ODE. This also makes clear that a two-level element leads only to an (uninteresting) single ODE.

Now the current through the 1–2 bond of the engine is given by

$$j_{12} = py - q \tag{7}$$

and hence in the stationary state the overall mean current through the elementary engine is

$$J = \frac{1}{2\tau}\int_0^{2\tau} j_{12}(t)\,\mathrm{d}t. \tag{8}$$

Let us now consider the time evolution of the current j_{12} during a half-period (time when $T =$ constant. Introducing the new variable $s = q + \frac{1-y}{1-x}p$, the equations for p and s during the half-period decouple:

$$\begin{aligned}\dot{p} &= 1 - (1 + x + y)p \\ \dot{s} &= \left(1 + \frac{1-y}{1-x}\right) - (2 + y)s.\end{aligned} \tag{9}$$

From equation (7) it follows that $j_{12} = p(y + \frac{1-y}{1-x}) - s$. Furthermore, the solutions to equation (9) for both half-periods (denoted by the indices $i = 1, 2$) have the same form:

$$\begin{aligned}p_i(t) &= p_{i0}\mathrm{e}^{-A_i t} + \frac{1}{A_i}(1 - \mathrm{e}^{-A_i t}) \\ s_i(t) &= s_{i0}\mathrm{e}^{-B_i t} + \frac{C_i}{B_i}(1 - \mathrm{e}^{-B_i t})\end{aligned} \tag{10}$$

where the coefficients $A = 1 + x + y$, $B = 2 + y$ and $C = 1 + (1 - y)/(1 - x)$ are to be evaluated at the corresponding T_i. The values of p_0 and s_0 at the beginning of a half-period can be obtained for the stationary situation by noticing that after a full period the values of p and s return to p_0 and s_0, so that:

$$p_{10} = \frac{(1 - \mathrm{e}^{-A_1\tau})\mathrm{e}^{-A_2\tau}/A_1 + (1 - \mathrm{e}^{-A_2\tau})/A_2}{1 - \mathrm{e}^{-(A_1+A_2)\tau}} \tag{11}$$

and

$$s_{10} = \frac{(1 = \mathrm{e}^{-B_1\tau})\mathrm{e}^{-B_2\tau}C_1/B_1 + (1 - \mathrm{e}^{-B_2\tau})C_2/B_2}{1 - \mathrm{e}^{-(B_1+B_2)\tau}}. \tag{12}$$

The values of p_{20} and s_{20} can be obtained from equations (11) and (12) by interchanging the indices 1 and 2, on the right-hand side. The mean current during the half-period $J_i = \tau^{-1}\int_0^\tau j(t)\,\mathrm{d}t$ is

$$\begin{aligned}J_i = \frac{1}{\tau}\left[\left(\frac{p_{i0}}{A_i} - \frac{1}{A_i^2}\right)(1 - \mathrm{e}^{-A_i\tau})(B_i + C_i - 3) - \left(\frac{s_{i0}}{B_i} - \frac{C_i}{B_i^2}\right)(1 - \mathrm{e}^{-B_i\tau})\right] \\ + \frac{(B_i + C_i - 3)}{A_i} - \frac{C_i}{B_i}\end{aligned} \tag{13}$$

and the overall mean current obeys $J = (J_1 + J_2)/2$. Note that the first term in equation (13) is due to a transient component of the current, while the last two are steady-state terms and correspond to the mean current caused by the outer potential difference, U. The explicit, tedious but otherwise elementary calculation of J as a function of T_1, T_2 and τ can be entrusted to MATHEMATICA.

The overall principle of the engine's work can be easily visualized in the limiting case of $T_1 \to \infty$ and $T_2 \to 0$. At the end of the cold half-period only sites 1 and 1′ are occupied. At the beginning of the hot half-period the occupation of all sites starts to equilibrate. This equilibration process does not lead to any net current for $k_B T_1 \gg \Delta E$, because then the system is essentially symmetric, since the small energy differences between sites do not play any role. After cooling the system again, the particles from site 3 go to the right and to the left with equal probabilities, while those from site 2 go only to the left; this gives rise to an overall net current from 2 to 1. This picture also makes clear that, as stated above, a spatially symmetric two-level ratchet cannot produce any current.

3. Net current, work and efficiency of the engine

Let us now discuss the results of the above equations. We start by considering the case $U = 0$ and the current flowing in the system; this situation is identical to a short-circuited three-level system. From equation (13) one infers readily that for fixed T_1 and T_2 the short-circuit current, J, is negative, that it tends to a constant value for $\tau \to 0$ and that it decays as $J \propto \tau^{-1}$ for large τ. The last feature is a clear signature of the essentially non-equilibrium nature of the heat engine considered: it works not because it is a non-ideal approximation to some absolutely reversible, quasistatic engine, but essentially because it is not quasistatic and irreversible.

Let us first consider the temperature dependence of the current. For this we fix the value of τ and consider J as a function of T_1 and T_2. Note that our dichotomous prescription, equation (3), is (by an appropriate choice of the origin) symmetric under time-inversion. The mean short-circuit current is invariant under this transformation. This means that for small temperature differences $\Delta T = T_1 - T_2$ the current must be an even function of ΔT, a clear sign of irreversibility. In fact for small ΔT one has in general $J \propto (\Delta T)^2$, a finding which is true in our case. We checked this explicitly, i.e. by showing from the general forms for $J(T_1, T_2, \tau)$, that for $T_1 = T_2 = T$ both J and its two partial derivatives with respect to T_1 and T_2 vanish.

The process that allows an elementary engine to work can be called a non-equilibrium directed diffusion (directed diffusion in a temperature field which is homogeneous in space but changing in time). This process is very different from a stationary thermodiffusion situation, in which the temperature bath is constant in time but inhomogeneous in space.

After the calculation of the mean current we are in the position to evaluate the power of the engine $P = -JU$ (the minus sign corresponds to the fact that the engine produces net work when the current flows to the left, against the potential difference U) and its efficiency $\eta = A/Q_1$, where $A = 2P\tau$ and Q_1 is the heat absorbed from the warmer reservoir. Neglecting all losses not connected with the work we have $Q_1 = A + \Delta\mathcal{E}$, where $\Delta\mathcal{E}$ is the change in the internal energy of the system during the half-period at the higher temperature T_1. The internal energy, $\mathcal{E}$, of the system equals $\mathcal{E} = (q + 2r)\Delta E = (2 - 2p - q)\Delta E$, and it can be easily evaluated. We find:

$$\Delta\mathcal{E} = [(3 - C_1)(p_{10} - p_{20}) + (s_{10} - s_{20})]\Delta E. \tag{14}$$

In figure 2 we present the power of the engine as a function of U for the values of parameters $\tau = 1$, $T_1 = 10$ and $T_2 = 0.5, 0.7, 1.0$. Notice that the power is negative for all negative U and for large positive U, and it is positive in between. This is the region of

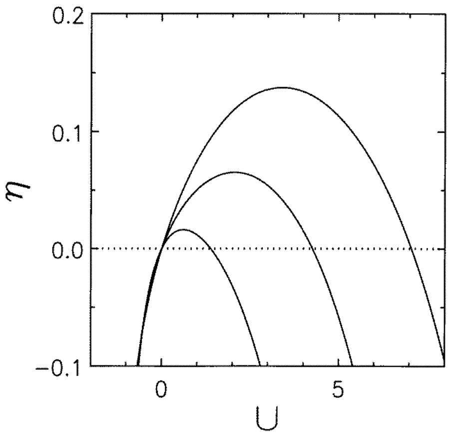

Figure 2. The power, P, of the elementary engine as a function of the potential difference, U. The three curves correspond to $T_2 = 0.5, 0.7, 1.0$, from top to bottom, see text for details.

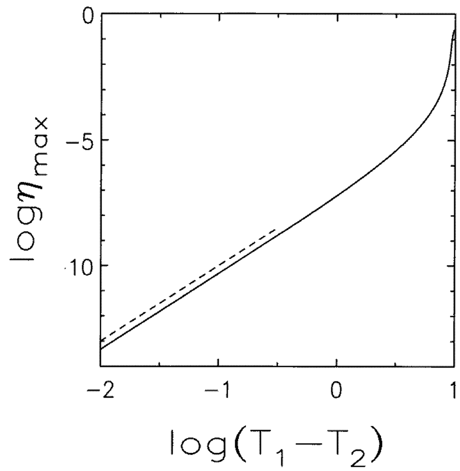

Figure 3. The maximal efficiency, $\eta_{\max}$, of the engine as a function of $T_1 - T_2$. Note the double-logarithmic scales. The broken line has a gradient of 3.

parameters in which the engine produces work. Outside this region the engine works as a 'heat transporter': it uses the temperature modulation to enhance the heat transport from the warm to the cold heat reservoir. In the region where it produces positive work the overall dependence of A on U shows a nearly parabolic behaviour, see figure 2, going through zero at $U = 0$ and attaining a maximum at a (positive) value U^*. Increasing the temperature difference renders this maximum higher and shifts it to larger U^* values. A similar picture obtains the efficiency, η, of the engine. In figure 3 we show the behaviour of the maximal η, $\eta_{\max}$ as a function of $\Delta T = T_1 - T_2$. The maximal efficiency grows as ΔT^3 for small ΔT (which is also very different from the reversible case where, according to the Carnot's formula, $\eta_{\max} \propto \Delta T$). For large ΔT the efficiency tends rapidly to a finite value. For fixed T_2 and τ this value does not tend monotonously to 1, as it would for a Carnot-engine, but rather to a smaller limiting value η^*, which is engine-specific. An interesting feature is the surprisingly strong dependence of η^* on T_2 for fixed T_1: our machine needs a very cold cooler rather than a very hot heater. Maximizing the value of η with respect to τ for fixed T_1 and T_2 we find, for example, that for $T_1 = 10$ and $T_2 = 1$ $\eta_{\max} = 0.196$ (compared with the Carnot value of $\eta_{\max} = 0.9$); the low value of the attainable $\eta_{\max}$ is a clear sign of irreversibility. Moreover, the maximum is attained for small values of the period 2τ, far from the quasistatic mode of the operation.

4. Conclusions

To conclude, we summarize the findings of our present work. We have presented a simple 'minimal' model for a thermally driven ratchet, namely an array of three-level elements switched in succession. We considered the behaviour of this system under thermal, parametrical modulations. We calculated the net current, work and efficiency of the elementary engine as functions of the upper and lower temperatures and of the modulation period. The temperature dependencies obtained differ largely from those of typical, quasistatically working heat engines. Furthermore, we discussed the general properties of the model and the connection to the inherently irreversible nature of the underlying process.

Acknowledgments

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