Directed transport by pumping of excited states

B. Cleuren and C. Van den Broeck
Limburgs Universitair Centrum, B-3590 Diepenbeek, Belgium
(Received 4 March 2002; published 12 July 2002)

We present the exact analytic solution for the model of directed transport induced by nonequilibrium state occupation, introduced by Porto [Eur. Phys. J. B **25**, 345 (2002)].

DOI: 10.1103/PhysRevE.66.012101 PACS number(s): 05.60.Cd, 05.40.−a, 87.16.Nn

I. INTRODUCTION

Brownian motors are small-sized objects capable of rectifying thermal fluctuations [1]. Directed transport results from a combination of broken spatial symmetry with nonequilibrium constraints that destroy detailed balance. Here, we focus on a recently introduced simple model [2], in which the nonequilibrium state is achieved by pumping of an excited state. We present a streamlined version of the model, encompassing all the key features, and derive analytical expressions for the velocity and diffusion coefficient using a general random walk formalism [3].

The model consists of two interacting particles, both performing a hopping motion in an equipotential lattice. The interaction prevents the particles from occupying the same site, or from being separated by more than one site. In other words, the two particles form a diatomic molecule that can be in two different states, say A and B, corresponding to the particles being either in nearest neighbor sites, or separated by one intermediate empty site. These *ground states* are separated by a potential barrier of height Δ. They are further supplemented with an excited state $A^\star$ of the nearest neighbor state A. This excited state can be reached from both states A and B. The energy difference between A and $A^\star$ will be called ϵ. An asymmetry is introduced in the transitions between B and $A^\star$. If the transition happens by a jump of the left particle, the barrierheight equals $\Delta\pm\epsilon$ ($+$ and $-$ sign, respectively, when the transition is to or from the excited state). However, when the right particle makes the jump, the barrierheight is $\Delta'\pm\epsilon$. Figure 1(a) shows all the transitions between the different states. The nonequilibrium condition is generated by pumping the transitions between A and $A^\star$. We will represent this effect by an energy parameter η, which effectively changes the energy difference, for transitions between A and $A^\star$, from ϵ to $\epsilon+\eta$. When $\eta<0$, transitions from A to $A^\star$ are facilitated, while for $\eta>0$ they are suppressed.

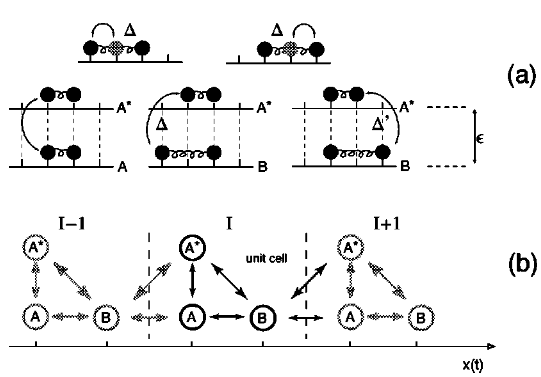

FIG. 1. (a) Schematic representation of the different states and their transitions. For each transition, the corresponding potential barrier height is shown. (b) Periodically repeated unit cell, consisting of three internal states.

II. ANALYTIC SOLUTION

Since the particles are separated by at the most one site, one needs not to give the separate positions $x_1(t)$ and $x_2(t)$ of both particles. It suffices to specify the configuration σ, namely, (A, $A^\star$, or B), and the *center of mass* $x(t)\equiv[x_1(t)+x_2(t)]/2$. For technical purposes it is more convenient to specify the state of the system by considering the periodic structure shown in Fig. 1(b). The coordinates of the system in this structure are $\sigma\in\{A,A^\star,B\}$ and the cell coordinate I. The center of mass then follows as $x=x_{\sigma,I}=I+\frac{1}{2}\delta_{\sigma,B}$. Assuming Markovian dynamics, the probability $P_{\sigma,I}(t)$ to find the system in state (σ,I) at time t satisfies the following master equation:

$$\begin{aligned}
\frac{\partial}{\partial t}P_{A,I}(t)=&-(k^-_{A\to B}+k^+_{A\to B}+k_{A\to A^\star})P_{A,I}(t)\\
&+k^+_{B\to A}P_{B,I-1}(t)+k^-_{B\to A}P_{B,I}(t)\\
&+k_{A^\star\to A}P_{A^\star,I}(t),\\
\frac{\partial}{\partial t}P_{A^\star,I}(t)=&-(k^-_{A^\star\to B}+k^+_{A^\star\to B}+k_{A^\star\to A})P_{A^\star,I}(t)\\
&+k^+_{B\to A^\star}P_{B,I-1}(t)+k^-_{B\to A^\star}P_{B,I}(t)\\
&+k_{A\to A^\star}P_{A,I}(t),\\
\frac{\partial}{\partial t}P_{B,I}(t)=&-(k^-_{B\to A}+k^+_{B\to A}+k^-_{B\to A^\star}-k^+_{B\to A^\star})P_{B,I}(t)\\
&+k^+_{A\to B}P_{A,I}(t)+k^-_{A\to B}P_{A,I+1}(t)\\
&+k^+_{A^\star\to B}P_{A^\star,I}(t)+k^-_{A^\star\to B}P_{A^\star,I+1}(t).
\end{aligned}\qquad(1)$$

Here, $k^\pm_{\sigma\to\omega}$ is the transition rate per unit time to go from state σ to state ω with a jump either to the left ($-$) or to the right ($+$). In concordance with the discussion given in the Introduction, these transition rates are taken to be of the Arrhenius type:

$$k^\pm_{A\to B}=k^\pm_{B\to A}=e^{-(\beta/2)\Delta},$$

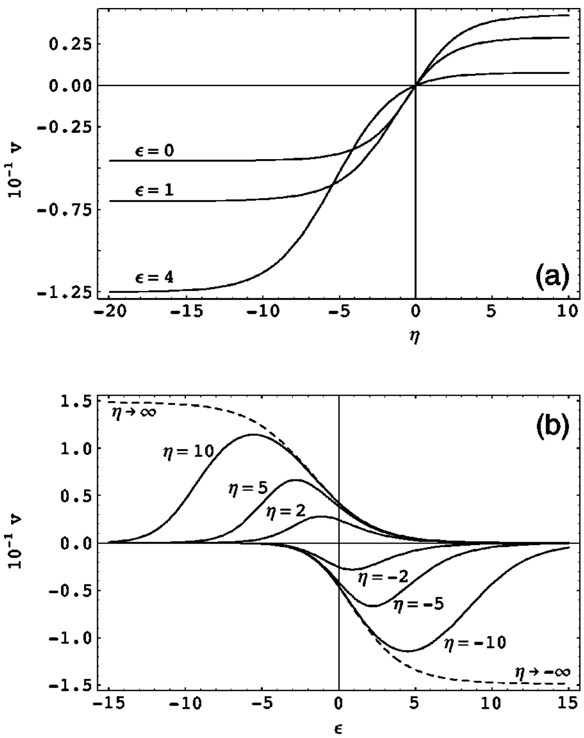

FIG. 2. (a) Plot of the average velocity v as a function of η for different values of ϵ. (b) Plot of v as a function of ϵ for different values of η. In both cases $k_BT=1$ and $\Delta=1$, $\Delta'=2$.

$$k_{A\to A^\star}=(k_{A^\star\to A})^{-1}=e^{-(\beta/2)(\epsilon+\eta)},$$

$$k^-_{A^\star\to B}=e^{-(\beta/2)(\Delta-\epsilon)};\quad k^+_{B\to A^\star}=e^{-(\beta/2)(\Delta+\epsilon)},\tag{2}$$

$$k^+_{A^\star\to B}=e^{-(\beta/2)(\Delta'-\epsilon)};\quad k^-_{B\to A^\star}=e^{-(\beta/2)(\Delta'+\epsilon)}.$$

In the following we will set $\beta=(k_BT)^{-1}=1$, defining the unity of energy.

Our main focus now is on the transport properties, namely, on the average velocity v:

$$v=\lim_{t\to\infty}\frac{\langle x(t)\rangle}{t},\tag{3}$$

and the diffusion coefficient D:

$$D=\lim_{t\to\infty}\frac{\langle x(t)^2\rangle-\langle x(t)\rangle^2}{t}.\tag{4}$$

These quantities can be calculated using the general formalism for random walks in periodic structures, cf. [3]. As far as the average speed v is concerned, the calculation is in fact very simple and we reproduce it here. Since $v=\lim_{t\to\infty}(\partial/\partial t)\langle x(t)\rangle$ with $\langle x(t)\rangle=\Sigma_{\sigma,I}x_{\sigma,I}P_{\sigma,I}(t)$, we obtain by multiplying the master equation (1) with $x_{\sigma,I}$ followed by summation over σ,I that

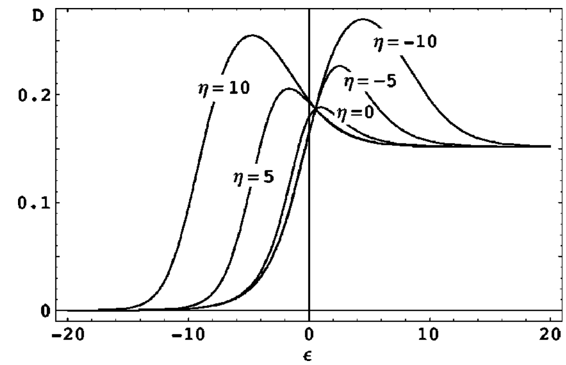

FIG. 3. Plot of the diffusion coefficient D as a function of ϵ for different values of η. Again $k_BT=1$ and $\Delta=1$, $\Delta'=2$.

$$v=(k^+_{B\to A}+k^+_{B\to A^\star})P^{st}_B-(k^-_{A\to B}P^{st}_A+k^-_{A^\star\to B}P^{st}_{A^\star}),\tag{5}$$

where $P^{st}_\sigma=\lim_{t\to\infty}\Sigma_I P_{\sigma,I}(t)$ is the steady state probability to be in state σ. The evolution equation for $P_\sigma(t)=\Sigma_I P_{\sigma,I}(t)$ is obtained by summing both sides of the master equation. The problem of finding the steady state solution is thus reduced to an algebraic problem, i.e., finding the eigenvector of eigenvalue 0 of the resulting transition matrix. One obtains

$$P^{st}_{A^\star}=\frac{e^{-\epsilon}}{Z}(e^{\Delta}+2e^{(1/2)(\Delta+\epsilon+\eta)}+e^{(1/2)(\Delta+\Delta')}+2e^{(1/2)(\epsilon+\eta+\Delta')}+2e^{(1/2)(\Delta+\epsilon+\Delta')}),$$

$$P^{st}_{A}=\frac{1}{Z}(e^{(\Delta+\eta)}+2e^{(1/2)(\Delta+\epsilon+\eta)}+e^{(1/2)(\Delta+2\eta+\Delta')}+2e^{(1/2)(\epsilon+\eta+\Delta')}+2e^{(1/2)(\Delta+\epsilon+2\eta+\Delta')}),\tag{6}$$

$$P^{st}_{B}=\frac{1}{Z}(e^{\Delta}+2e^{(1/2)(\Delta+\epsilon+\eta)}+e^{(1/2)(\Delta+\Delta')}+2e^{(1/2)(\epsilon+\eta+\Delta')}+2e^{(1/2)(\Delta+\epsilon+2\eta+\Delta')}),$$

where Z is determined by normalization. Combined with Eq. (5), it yields the central result:

$$v=\frac{e^{\epsilon}(1-e^{\eta})(1-e^{(1/2)(\Delta'-\Delta)})}{(e^{(1/2)\Delta}+e^{(1/2)\Delta'}+e^{[(1/2)\Delta+\epsilon]}+e^{[\epsilon+(1/2)\Delta']}+e^{[(1/2)\Delta+\epsilon+\eta]}+e^{[\epsilon+\eta+(1/2)\Delta']}+2e^{(1/2)(\epsilon+\Delta')}+2e^{(1/2)(\epsilon+\eta)}+2e^{(1/2)(\epsilon+\eta+\Delta'-\Delta)}+4e^{(1/2)(3\epsilon+\eta)}+4e^{(1/2)(3\epsilon+\eta+\Delta'-\Delta)}+4e^{(1/2)(3\epsilon+2\eta+\Delta')})}.\tag{7}$$

In the absence of pumping, $\eta=0$, the steady state solution reduces to the well known Gibbsian form for the equilibrium distribution, and the flux vanishes, $v=0$. The extremal values of the fluxes, on the other hand, are found in the limits of overpopulation $\eta\to-\infty$ and underpopulation $\eta\to\infty$, namely:

$$v \overset{\eta\to\infty}{=} -(e^{\Delta/2}-e^{\Delta'/2})/(e^{\Delta}+e^{(\Delta+\Delta')/2}+4\,e^{(\Delta+\epsilon+\Delta')/2}),$$

$$v \overset{\eta\to-\infty}{=} e^{\epsilon}(e^{\Delta/2}-e^{\Delta'/2})/(e^{\Delta}+e^{(\Delta+\Delta')/2}+2e^{(\Delta+\epsilon+\Delta')/2}+e^{(\Delta+2\epsilon+\Delta')/2}+e^{\Delta+\epsilon}). \tag{8}$$

Figure 2 shows the dependence of v on η and ϵ for the values of $\Delta=1$ and $\Delta'=2$. The results are in qualitative agreement with the numerical results presented in Ref. [2]. The differences arise from the fact that we choose to work with the more realistic case of a continuous time model, whereas the results in Ref. [2] are obtained for a discrete time variable.

The calculation of D is much more elaborate, and we refer to Ref. [3] for more details. The final result is lengthy and reproduced in the Appendix. Here we only quote the result for the diffusion coefficient in the absence of pumping:

$$D=\frac{e^{(1/2)(-\Delta+\epsilon)}(e^{\Delta}+e^{(\epsilon+\Delta/2)}+e^{(\Delta+\epsilon/2)}+2e^{(1/2)(\Delta+\epsilon)}+e^{(\epsilon+\Delta'/2)}+e^{(1/2)(\Delta+\epsilon+\Delta')}+e^{(1/2)(\Delta+2\epsilon+\Delta')})}{(1+2e^{\epsilon})(e^{\Delta}+2e^{(1/2)(\Delta+\epsilon)}+e^{(1/2)(\Delta+\Delta')}+2e^{(1/2)(\epsilon+\Delta')}+2e^{(1/2)(\Delta+\epsilon+\Delta')})}. \tag{9}$$

In Fig. 3 we show the dependence of D on η and ϵ for the values of $\Delta=1$ and $\Delta'=2$.

III. DISCUSSION

The calculation of drift and diffusion properties for models of Brownian motors with a finite number of discrete states can be reduced to a problem of linear algebra. The calculation of the drift velocity is particularly simple since it only requires the knowledge of a steady state probability distribution. Many of these models can thus be solved exactly, independently of whether or not detailed balance holds. As such, the description with discrete states has an important advantage over models with continuous degrees of freedom, since steady state properties can usually no longer be obtained for more than one degree of freedom in the absence of detailed balance.

APPENDIX

$$\begin{aligned}
D=&\frac{1}{2}e^{(1/2)(-\Delta+\epsilon)}[e^{\Delta/2}-e^{\Delta'/2}]\bigg\{(e^{\Delta}+e^{\Delta+\epsilon/2+\eta}+2e^{(1/2)(\Delta+\epsilon+\eta)}+2e^{(1/2)(\epsilon+\eta+\Delta')}+e^{(1/2)(\Delta+\Delta')}+2e^{(1/2)(\Delta+2\epsilon+\eta)}\\
&+2e^{(1/2)(\Delta+\epsilon+\Delta')}+2e^{(1/2)(\Delta+2\epsilon+2\eta+\Delta')}+2e^{(1/2)(2\epsilon+\eta+\Delta')}+e^{(1/2)(\Delta+\epsilon+2\eta+\Delta')}]\\
&\times(2e^{(2\Delta+\epsilon+\eta)/2}(2+4e^{\epsilon}+e^{2\epsilon})+(e^{3\Delta/2}+2e^{\Delta+3(\epsilon+\eta)/2})(1+e^{\epsilon})+e^{\Delta/2+\epsilon+\eta}(4+8e^{\epsilon}+2e^{\Delta}+e^{\Delta+\epsilon})+e^{3\Delta/2+2\epsilon+2\eta}\\
&+e^{(\Delta'/2)}\{e^{\Delta+2(\epsilon+\eta)}(1+2e^{\epsilon/2})+(e^{\Delta}+2e^{\Delta+\epsilon/2}+2e^{[\Delta+3(\epsilon+\eta)]/2})(1+e^{\epsilon})+2e^{(\Delta+\epsilon+\eta)/2}(2+2e^{\epsilon/2}+4e^{\epsilon}+4e^{3\epsilon/2}+e^{2\epsilon})\\
&+e^{\epsilon+\eta}[4+e^{\Delta}(1+2e^{\epsilon/2})(2+e^{\epsilon})+8e^{\epsilon}]\})+e^{\epsilon}[e^{\Delta}+2e^{(1/2)(\Delta+\epsilon+\eta)}+e^{(1/2)(\Delta+\Delta')}+2e^{(1/2)(\epsilon+\eta+\Delta')}+2e^{(1/2)(\Delta+\epsilon+2\eta+\Delta')}]\\
&\times\bigg(2(1+3e^{\epsilon}+e^{3\epsilon/2})e^{\Delta+\epsilon/2+3\eta/2}+e^{3\Delta/2}(1+e^{\epsilon/2})(1+e^{\epsilon})-e^{(\Delta+\epsilon)/2+\eta}[4+e^{\epsilon}(8-e^{\Delta})-e^{(\epsilon/2)}(8+e^{\Delta})-16e^{3\epsilon/2}]\\
&+e^{\Delta'/2}\{2e^{\Delta+3\epsilon/2+2\eta}(1+e^{\epsilon/2})+e^{\Delta}(1+e^{\epsilon/2})(1+e^{\epsilon})+2e^{(\Delta+3\eta)/2}(e^{\epsilon/2}+4e^{\epsilon}+3e^{3\epsilon/2}+9e^{2\epsilon})+e^{\epsilon/2+\eta}[-4+2e^{\Delta}+2e^{3\epsilon/2}\\
&\times(8+e^{\Delta})+e^{\epsilon}(-8+3e^{\Delta})+e^{(\epsilon/2)}(8+3e^{\Delta})]-2e^{(1/2)(\Delta+\eta)}(1+e^{\epsilon}+e^{(3/2)\epsilon}-e^{2\epsilon})\}-2e^{\Delta+\epsilon+\eta/2}\bigg[1-5\cosh\left(\frac{\epsilon}{2}\right)-\sinh\left(\frac{\epsilon}{2}\right)\\
&-2\sinh(\epsilon)\bigg]\bigg)\bigg\}\bigg/\;[e^{\Delta}+e^{\Delta+\epsilon}+2e^{(1/2)(\Delta+\epsilon+\eta)}+2e^{(1/2)(\Delta'+\epsilon+\eta)}+e^{\Delta+\epsilon+\eta}+4e^{(1/2)(\Delta+3\epsilon+\eta)}+4e^{(1/2)(\Delta'+3\epsilon+\eta)}\\
&+e^{(1/2)(\Delta+\Delta')}+2e^{(1/2)(\Delta+\Delta'+\epsilon)}+e^{(1/2)(\Delta+\Delta'+2\epsilon)}+e^{(1/2)(\Delta+\Delta'+2\epsilon+2\eta)}+4e^{(1/2)(\Delta+\Delta'+3\epsilon+2\eta)}]^{3}+\tfrac{1}{2}\,e^{\epsilon}[e^{-\Delta/2}+e^{-(\epsilon+\Delta)/2}\\
&-v][e^{\Delta}+2e^{(1/2)(\Delta+\epsilon+\eta)}+e^{(1/2)(\Delta+\Delta')}+2e^{(1/2)(\epsilon+\eta+\Delta')}+2e^{(1/2)(\Delta+\epsilon+2\eta+\Delta')}]/[e^{\Delta}+e^{\Delta+\epsilon}+2e^{(1/2)(\Delta+\epsilon+\eta)}\\
&+2e^{(1/2)(\Delta'+\epsilon+\eta)}+e^{\Delta+\epsilon+\eta}+4e^{(1/2)(\Delta+3\epsilon+\eta)}+4e^{(1/2)(\Delta'+3\epsilon+\eta)}+e^{(1/2)(\Delta+\Delta')}+2e^{(1/2)(\Delta+\Delta'+\epsilon)}+e^{(1/2)(\Delta+\Delta'+2\epsilon)}\\
&+e^{(1/2)(\Delta+\Delta'+2\epsilon+2\eta)}+4e^{(1/2)(\Delta+\Delta'+3\epsilon+2\eta)}].
\end{aligned}$$

[1] M.O. Magnasco, Phys. Rev. Lett. **71**, 1477 (1993); F. Jülicher and J. Prost, Prog. Theor. Phys. Suppl. **130**, 9 (1998); C. Van den Broeck, P. Reimann, R. Kawai, and P. Hänggi, in *Statistical Mechanics of Biocomplexity*, edited by D. Reguera, J. M. G. Vilar, and J. M. Rubi (Springer-Verlag, 1999), pp. 93-111; P. Reimann, Phys. Rep. **361**, 57 (2002).
[2] M. Porto, Eur. Phys. J. B **25**, 345 (2002).
[3] I. Claes and C. Van den Broeck, J. Stat. Phys. **70**, 1215 (1993).