Collective particle transport in a peristaltic ratchet system

Marcel Dierl[1], Mario Einax[1], Petr Chvosta[2], Wolfgang Dieterich[3] and Philipp Maass[1]

[1] Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany
[2] Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, CZ-180 00 Praha, Czech Republic
[3] Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

E-mail: marcel.dierl@uos.de

Abstract. We consider particles with repulsive nearest-neighbor interactions in a periodically modulated tilted-sine potential as a model for a peristaltic ratchet system. Using the Markov chain approach to kinetics (MCAK), the collective transport behavior is investigated with respect to the modulation period, interaction strength, and applied mechanical bias (tilt amplitude). In the stationary state, a maximum is found in the period-averaged particle current and transport efficiency as function of both the mechanical bias and the modulation period. The efficiency can be enhanced when the interaction strength is increased. While the maximal current arises for fast modulation, maximum efficiency is obtained for comparatively slow modulation.

1. Introduction

Active transport plays an important role in biological processes at the cellular level. A typical example is the sodium-potassium ATPase in living cells, which drives the ions against a chemical gradient. Theoretical studies of such biological transport processes are often based on models, where transport of particles against the gradient is induced by a time-dependent potential without spatial inversion symmetry. Insights into driving mechanisms have been gained by studying Brownian dynamics of single particles [1, 2] or many-particle hopping models with hard-core exclusions [3, 4]. On the basis of analytical approaches, extensions of these treatments towards interparticle interactions beyond hard-core exclusions are difficult. Recently, it has been shown for a two-site model that such interactions can successfully be treated by time-dependent density functional theory (TDFT) [5].

Inspired by these studies, we apply the Markov chain approach to kinetics (MCAK) [6] to a many-particle ratchet model. In this approach, which is equivalent to the TDFT, exact equilibrium relations between correlation functions and densities on a local scale are derived from Markov chains. The merits of the MCAK over the TDFT are discussed in [6]. In the model, particles with repulsive nearest-neighbor interactions are driven by a traveling sine wave against a bias in a channel that is coupled to two particle reservoirs. Applying the MCAK, a closed set of kinetic equations for the collective particle flow is derived. By numerical solution of these equations we obtain the stationary current in and the efficiency of the ratchet as a function of the modulation period as well as the interaction and bias strength.

2. Model

The channel is considered to be composed of N sites, where each site i is either occupied by a particle (occupation number $n_i = 1$) or vacant ($n_i = 0$). Particles can be ejected to and injected from two reservoirs L and R, as sketched in Figure 1(a). Applying the equilibrated-bath couplings from [5, 6, 7, 8], the reservoir influence on the injection and ejection rates is determined by the chemical potentials $\mu_{\rm L}$ and $\mu_{\rm R}$, such that the respective rates fulfill detailed balance conditions with respect to the grand canonical potentials belonging to $\mu_{\rm L}$ and $\mu_{\rm R}$. This means that each reservoir tends to establish a corresponding equilibrium state. For the specific form of the injection and ejection rates, the exponential rates of Eq. 2 are used (see below). No interaction is considered between a particle inside the channel and a particle in a reservoir. Inside the channel, a repulsive nearest-neighbor interaction of strength $V > 0$ is present.

The reservoirs are assumed to have ("electro-")chemical potentials $\mu_{\rm L}$ and $\mu_{\rm R} + F$, where F corresponds to a constant bias, i.e. $\varepsilon_{i+1}^{(\rm s)} - \varepsilon_i^{(\rm s)} = F/(N+1)$. Here the superscript indicates the "static part" of the energy levels, $\varepsilon_i^{(\rm s)} = \varepsilon_1^{(\rm s)} + F(i-1)/(N+1)$. Introducing the differences between the (static) boundary site energies and reservoir levels, $\Delta_{\rm L} = \varepsilon_1^{(\rm s)} - \mu_{\rm L}$ and $\Delta_{\rm R} = \mu_{\rm R} + F - \varepsilon_N^{(\rm s)}$, we can, without loss of generality, set $\mu_{\rm L} = 0$ in the following. Superimposed to the linearly increasing bias potential is a peristaltic driving mode, represented by a traveling sine wave with amplitude A and modulation period $\tau = 2\pi/\omega$. The site energies hence become

$$\varepsilon_i(t) = \varepsilon_1^{(\rm s)} + \frac{F}{N+1}(i-1) + A\left[1 + \sin\left(\frac{\pi}{2}\,i - \omega t\right)\right], \qquad i = 1, \ldots, N\,. \tag{1}$$

The jump rate of a particle from site i to a vacant neighboring site $f = i \pm 1$ is

$$\Gamma_{i,f}(t) \propto \exp\left[\frac{-\Delta E_{i,f}(t)}{2}\right], \tag{2}$$

where $\Delta E_{i,f}(t)$ denotes the energy difference between the final and initial state after and before the jump at time t; we here and in the following set the thermal energy as energy unit, i.e. $k_{\rm B}T = 1$.

3. Computational details

Using the master equation for the time evolution of the probability density $P(n_1, \ldots, n_N, t)$ of microstates, the evolution equations for the mean occupation numbers $\rho_i(t) \equiv \langle n_i \rangle_t = \sum_{\{n_i\}} n_i P(n_1, \ldots, n_N, t)$ are

$$\frac{{\rm d}\rho_i(t)}{{\rm d}t} = J_{i-1,i}(t) - J_{i,i+1}(t)\,, \tag{3}$$

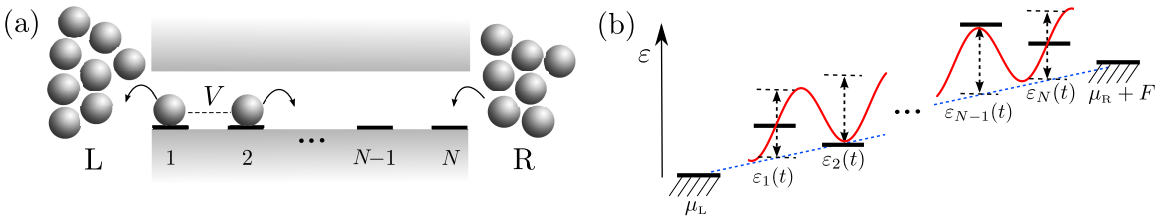

Figure 1. (a) Sketch of the model. (b) Visualization of the site energies with $\Delta_{\rm L} = \Delta_{\rm R} = F/(N+1)$ along the channel at time t.

with net currents $J_{i,i+1}(t) = j_{i,i+1}(t) - j_{i+1,i}(t)$ from site i to $(i+1)$. Applying the MCAK procedure to the ratchet model yields for the bulk currents $j_{i,i+1} = \langle n_i(1-n_{i+1})\Gamma_{i,i+1}\rangle_t$ the analytical form [9]

$$j_{i,i+1} = \left[(\rho_{i+2} - C_{i+1})e^{-V/2} + \tilde{\rho}_{i+1} - \rho_{i+2} + C_{i+1}\right] \frac{\rho_i - C_i}{\rho_i \tilde{\rho}_{i+1}} \left[\rho_i - C_{i-1} + e^{V/2} C_{i-1}\right] e^{(\varepsilon_i - \varepsilon_{i+1})/2}, \tag{4}$$

where $\tilde{\rho}_i = 1 - \rho_i$ and C_i follows from the quadratic equation [10]

$$C_i = \exp(-V) \frac{(\rho_i - C_i)(\rho_{i+1} - C_i)}{1 - \rho_i - \rho_{i+1} + C_i}. \tag{5}$$

Similar expressions are obtained for the injection and ejection rates [6]. Solving Eq. (5) for the C_i as functions of ρ_i and ρ_{i+1}, and inserting into Eq. (4), yields the currents as functions of the mean occupation numbers. In this way, the kinetic equations (3) become a closed set.

Numerical integration of this set allows us to discuss the output power and performance of the device. Let us denote an averaging of an observable $A(t)$ over one period in the stationary regime by $\bar{A}$, i.e. $\bar{A} = \lim_{t_0\to\infty} \tau^{-1} \int_{t_0}^{t_0+\tau} \mathrm{d}t A(t)$. The mean number of particles transported by the ratchet per period is $\bar{J} = \bar{J}_{i,i+1}$, and accordingly the mean output power becomes $\bar{P}_{\mathrm{out}} = \bar{J}F$. The mean work done on the machine per period is $\bar{P}_{\mathrm{in}} = \overline{\sum_{i=1}^{N} \rho_i \dot{\varepsilon}_i}$, where $\dot{\varepsilon}_i(t) = \mathrm{d}\varepsilon_i(t)/\mathrm{d}t$. Accordingly we can define the efficiency of the machine by

$$\eta = \frac{\bar{P}_{\mathrm{out}}}{\bar{P}_{\mathrm{in}}} = \frac{\bar{J}F}{\overline{\sum_{i=1}^{N} \rho_i \dot{\varepsilon}_i}}. \tag{6}$$

4. Results and discussion

In the calculations, the following choice of parameters is used: $N = 10$, $A = 5$, $\Delta_{\mathrm{L}} = F/(N+1) - 2$, and $\Delta_{\mathrm{R}} = F/(N+1) + 2$. Let us first take a look at the current $\bar{J}$ as a function of the modulation time τ. The solid line in Figure 2 shows results for $V = 1$ and $F = 10$ obtained from MCAK calculations. As can be seen from the figure, the current increases rapidly and goes through a maximum at $\tau \approx 0.9$. In order to test how well the MCAK captures the kinetics, we have performed also kinetic Monte Carlo (KMC) simulations of the ratchet model. The results are marked by the circles in Figure 2 and show a good agreement with the MCAK predictions. For details of the KMC algorithm with time-dependent transition rates, see [11, 12].

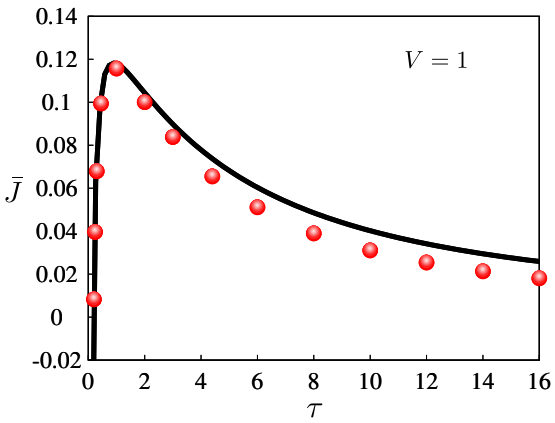

Figure 2. Average particle current $\bar{J}$ as function of τ for $V = 1$ and $F = 10$. The circles refer to results from KMC simulations.

In Figure 3 we analyze the performance of the ratchet model. The efficiency as function of the mechanical bias F is shown in Figure 3(a) for one representative driving period $\tau = 2$ and three different values $V = 0$, 1, and 10. All curves run through a maximum that increases and shifts to larger F values with increasing V. Figure 3(b) displays the efficiency as a function of the driving period. These curves again show a maximum of η that increases with V and shifts to

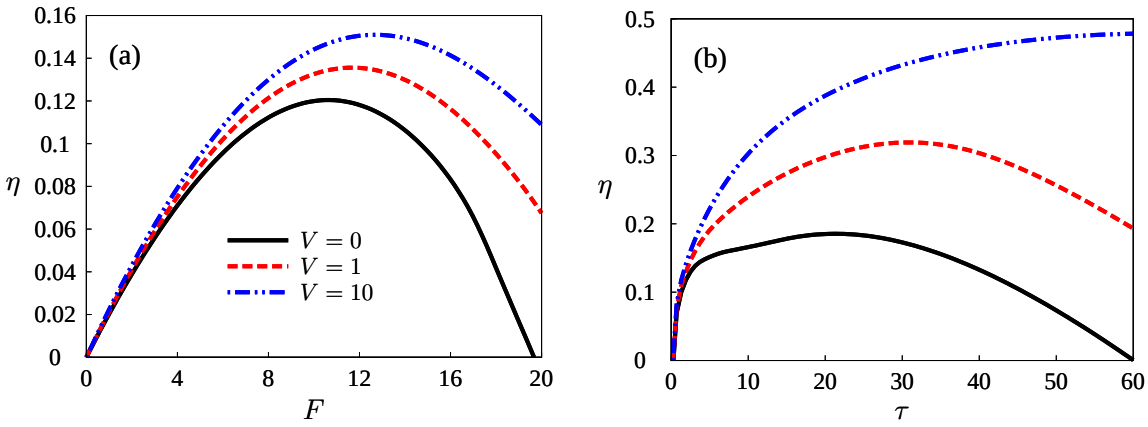

Figure 3. (a) Efficiency η as function of (a) mechanical bias F for $\tau = 2$ and (b) modulation period τ for $F = 10$. The assignment of lines to the different interaction strengths is given in (a).

larger τ. Accordingly, to keep η at maximum with increasing V, or decreasing temperature, the modulation of site energies needs to be slowed down.

Contrasting the finding in Figure 2, where maximal particle flow is obtained for fast modulation, highest efficiency is obtained for slow driving. These observations are reminiscent to those found for the minimal ratchet model ($N = 2$) studied in [5]. However, the present model with $N = 10$ shows much larger efficiencies for certain parameter choices, see, for example, the curve for $V = 10$ in Figure 3(b). This suggests that efficiencies for particle transport against a mechanical load are increased in longer channels.

In summary, our work has shown how the mechanical bias, the modulation period and the interaction strength affect the particle flow and the efficiency. It provides a guideline for optimizing this system.

Acknowledgments

We thank A. Nitzan for very illuminating discussions and acknowledge financial support from the German Academic Exchange Service DAAD (Grant No. 50755689).

References

[1] Reimann P 2002 *Phys. Rep.* **361** 57
[2] Hänggi P and Marchesoni F 2009 *Rev. Mod. Phys.* **81** 387
[3] Derényi I and Ajdari A 1996 *Phys. Rev. E.* **54** R5
[4] Aghababaie Y, Menon G I and Pliscke M 1999 *Phys. Rev. E* **59** 2578
[5] Einax M, Solomon G C, Dieterich W and Nitzan A 2010 *J. Chem. Phys.* **133** 054102
[6] Dierl M, Einax M and Maass P 2013 *Phys. Rev. E* **87** 062126
[7] Einax M, Dierl M and Nitzan A 2011 *J. Phys. Chem. C* **115** 21396
[8] Dierl M, Maass P and Einax M 2012 *Phys. Rev. Lett.* **108** 060603
[9] Dierl M, Maass P and Einax M 2011 *Europhys. Lett.* **93** 50003
[10] Buschle J, Maass P and Dieterich W 2000 *J. Phys. A: Math. Gen.* **33** L41
[11] Einax M and Maass P 2009 *Phys. Rev. E* **80** 020101(R)
[12] Holubec V, Chvosta P, Einax M and Maass P 2011 *Europhys. Lett.* **93** 40003