Commun. Comput. Phys.
doi: 10.4208/cicp.2009.09.123

Vol. 7, No. 5, pp. 904-926
May 2010

Investigation on Energetic Optimization Problems of Stochastic Thermodynamics with Iterative Dynamic Programming

Linchen Gong[1], Ming Li[2,*] and Zhong-can Ou-Yang[1,3]

[1] *Center for Advanced Study, Tsinghua University, Beijing, 100084, China.*
[2] *College of Physical Science, Graduate university of Chinese Academy of Sciences, Beijing, 100190, China.*
[3] *Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing, 100190, China.*

Received 24 July 2009; Accepted (in revised version) 8 October 2009

Available online 6 January 2010

Abstract. The energetic optimization problem, *e.g.*, searching for the optimal switching protocol of certain system parameters to minimize the input work, has been extensively studied by stochastic thermodynamics. In this work, we study this problem numerically using iterative dynamic programming. The model systems under investigation are toy actuators consisting of spring-linked beads with loading force imposed on both ending beads. For the simplest case, *i.e.*, a one-spring actuator driven by tuning the stiffness of the spring, we compare the optimal control protocol of the stiffness for both the overdamped and the underdamped situations, and discuss how inertial effects alter the irreversibility of the driven process and thus modify the optimal protocol. Then, we study the systems with multiple degrees of freedom by constructing oligomer actuators, in which the harmonic interaction between the two ending beads is tuned externally. With the same rated output work, actuators of different constructions demand different minimal input work, reflecting the influence of the internal degrees of freedom on the performance of the actuators.

PACS: 05.40.-a, 82.70.Dd, 87.15.H-, 05.70.Ln

Key words: Iterative dynamic programming, stochastic thermodynamics, harmonic model.

1 Introduction

The past two decades have seen the rapid growth of researches on nano-machines. Various types of nano-machines have been proposed and synthesized for practical purposes [1, 2]. This progress presents an urgent appeal and also a great challenge for

*Corresponding author. *Email address:* liming@gucas.ac.cn (M. Li)

physicists to understand the working principle and energetics of nano-machines. For isothermal nano-machines including protein machines and their derivatives or mimics, researchers are able to formulate a conceptual framework, the Brownian ratchet, to understand in general how a *scalar* energy source (light, chemical reaction, thermal agitation, etc.) can facilitate a *vectorial* process. The ratchet mechanism has not only been used to explain many experimental observations on chemically-driven protein motors [3–5], but also been successfully employed to develop some micro-manipulation techniques (*e.g.*, a ratchet-like micro-device was designed for DNA segregation [6]). Within the ratchet framework, the energetics (or thermodynamics) has also been extensively investigated with multiple-state Langevin equations or Fokker-Planck equations (*e.g.*, see [3] for chemically-driven nano-machines, and [7] for externally-controllable nano-machines).

In this context, some general energetic topics of nano-machines can be put forward. Particularly, in analogy to the optimization theory based on macroscopic finite-time thermodynamics [8,9], the energetic optimization problems can be re-formulated for ratchet-type nano-machines. For instance, one may require the *m*inimal *i*nput *w*ork (abbreviated as MIW) in a finite-time process to achieve least heat agitation [10] or maximum power [11] or highest efficiency [12]. To properly formulate these questions, choosing proper model systems is very important. While the multiple-state ratchet model may not be a proper candidate (especially, not easy for analytical treatment), Sekimoto and Seifert *et al.* initiated the study with a much simpler ratchet model. In this model, the machine performs Brownian motion on an energy landscape. And, a few parameters that characterize the landscape can be switched externally according to a deterministic protocol [11,15]. For such driven systems, stochastic thermodynamics has been firmly established, and the work and heat can be co-identified under the construction of first-law-like and second-law-like thermodynamic relations [15–17]. With the well-defined model systems and thermodynamics, a basic question is addressed, *i.e.*, what is the *o*ptimal *p*rotocol of the switching parameters to realize the *m*inimal *i*nput *w*ork (abbreviated as OPMIW). For the simple cases that the Brownian motion of an overdamped or underdamped bead is controlled by a tunable harmonic potential, the authors were able to present analytical solutions for the OPMIWs (see [11,13] for overdamped case, and [14] for underdamped case). While their analysis focused on analytically solvable potentials, Then and Engel also presented a Monte Carlo numerical method to discuss similar optimization problems of more complicated systems [10].

In this work, we follow the same logic and introduce a numerical method called *i*terative *d*ynamic *p*rogramming (abbreviated as IDP) [18] to investigate the OPMIW problems. For systems with polynomial potential functions up to the second order, the OPMIW problem is equivalent to the conventional optimal control problem, thus can be solved numerically with IDP. Inspired by the controllable DNA nano-actuator converting chemical energy into mechanical work [19,20], we choose toy actuators as our model systems. The simplest construction is a two-bead actuator, in which the two beads are linked by a spring with externally tunable stiffness (a polymer can be regarded as such an actuator if its persistence length is tuned externally). Although this model has been