Rotatory Molecular Machines: Dynamics, Power and Efficiency

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Cells are the minimum unit of life. They are systems out of equilibrium with a continuous active flux of energy and matter. The macromolecules in charge of such functions are the Molecular Machines, which are continuously transducing between energies of different nature. At first glance, these machines may look as its macroscopic counterpart, however, they live under a very different physical conditions. The scales involved provide very viscous dynamics which overcome the inertial effects. Additionally, the thermal energy is smaller but comparable to the rest of the energies involved in the motor cycle making thermal fluctuations essential in a proper description of such machines. Thus the dynamics of Molecular Machines can be addressed through an overdamped Langevin equation,

$$\gamma \dot{x} = -V'(x,t) + F_E + \xi(t). \tag{1}$$

Being x the spatial coordinate of the motor with an effective friction coefficientγ. The forces generating the motion are: the force induced by the motor through the internal motor potential $V(x,t)$, the thermal force $\xi(t)$, which can be described as a white noise and finally an the external force F_E. The aim of the theoretical study of Molecular Machines is to find the mechanism of transduction of the motor, i.e. the shape and dynamics of the motor potential. This is done by studying experimental trajectories under different experimental conditions and obtaining the different processes (mechanic and catalytic) composing the work cycle of the motor. The two main tunable experimental parameters are γ (attaching a passive load to the motor) and F_E which introduce respectively dissipative and conservative forces to the dynamics of the motor[1].

Molecular Motors are fueled by two different energy sources: The hydrolysis of nucleotides and a gradient of ions across a membrane, an example of a motor with both sources is F_0F_1ATPsynthase (Fig. 1). Specifically, the F_1 part can hydrolyze ATP to rotate its central shaft. From a study of the dependence of the motor with [ATP], and dissipative and conservative forces the motor potential has been successfully reconstructed and can be expressed as a flashing ratchet mechanism[1,2]. The resulting potential not only is able to reproduce the experimental observations through simulations but also allows an analytical insight of the structural configuration and how is related to optimizes the function of the motor[2,1,3]. The motor potential makes possible also to compute the power and the efficiency of the motor showing the importance of thermal fluctuations to study Molecular Machines[4].

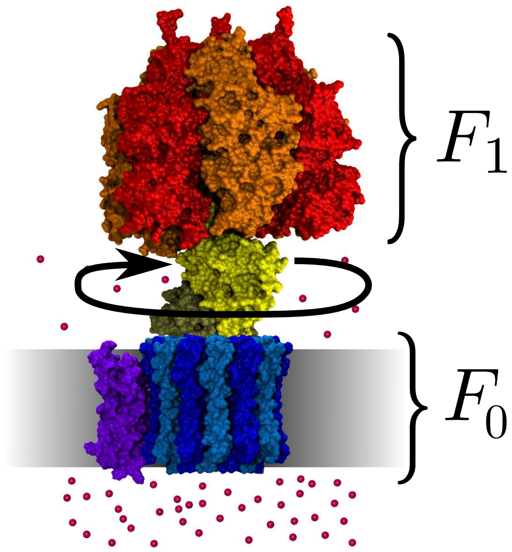

FIG. 1. F_0F_1 ATPsynthase is a molecular motor. The F_0 portion transduces a membrane flux into a rotation that is used by the F_1 subunit to synthesize ATP. It can also work in reverse mode, hydrolyzing ATP to generate membrane potential. Both subunits can be separated and work as individual motors working with a rotatory motion.

Alternatively, the basic mechanism for a molecular machine working with a flux of particles (as the F_0) allows the same formalism. Depending on the direction of the flux with respect to the particle gradient, this machine can work in both regimes turbine and pump. Setting out the most simple molecular flux machine of a piston under a Brownian force the dynamics of such a machine can be studied[5]. From the exact solution for the velocity of the motor and the flux, a new regime near the stall force arises where no useful energy can be obtained from the motor. This new regimes modifies completely the deterministic scenario for the power and the efficiency creating new maxima on account of the thermal fluctuations.

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