The theory of non-autonomous molecular motor motion.

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***Short Abstract* — Molecular motors are molecules capable of performing controlled mechanical motion. Motivated by recent experiments with nano-mechanical systems, which include both biological molecular motors and artificially synthesized molecules with rotational degrees of freedom, we discuss generic laws that describe response of an arbitrary nano-mechanical system to periodic modulation of control parameters. We formulate generic exact results, referred to as the Pumping-Quantization Theorem (PQT) and the Pumping-Restriction Theorem (PRT) that identify the conditions for, respectively, robust quantized behavior and for efficient control of a molecular machine. These theorems follow from the thermodynamic constraints and from the fact that the motion of a periodically driven molecular motor, interacting with thermal stochastic environment, is described by geometric phases analogous to the Berry phases in quantum mechanics.**

***Keywords* — molecular motors, mesoscopic thermodynamics.**

Alongside rapid progress revealing the details of biological motors such as kinesin and myosin, laboratories around the world have begun piecing together the components of artificial machines -- molecular rotors, gears, axles, and the like [1]. However, the outstanding problem to build an artificial molecular motor with efficiency comparable to biological molecules has not been solved. To guide the research on synthesis of new nano-mechanical systems, the additional theoretical insight is needed. Here we report about recent theoretical progress in understanding motion that can be induced at nano-scales by periodic in time control signals.

We can formalize the problem and model a molecular motor in noisy environment by a finite Markov chain, which can be represented as a graph. In such a graph, vertices correspond to discrete states of a molecule and links correspond to allowed transitions. Due to thermodynamic constraints, kinetic rates $k(j,i)$ of transitions from the state i to the state j satisfy the detailed balance condition and can be parametrized by parameters $E(i)$ (called well depths) and $W(i,j)=W(j,i)$ (barrier heights) such that $k(j,i)=\exp[E(i)-W(i,j)]$. Time-dependent control fields modulate these parameters and lead to directed motion of a system (the phenomenon is referred to as the pump effect [2]).

We found that the pump effect in noisy environment is described by geometric phases in evolution of the moment generating function of currents through links of a graph [2]. Moreover, due to thermodynamic constraints, this result can be generalized even to nonadiabatic control signals [3]. Following this theory, we derived the exact results, which can be applied to a generic nano-mechanical system [4,5].

The PRT makes two assertions:

(a) Pump currents through various links can be considered as vectors in a vector space whose dimension is equal to the maximum number of time-dependent barriers $W(i,j)$ such that removing the links, corresponding to these barriers, does not break the graph into disjoint components.

(b) Constraints on the pump currents predicted by the part (a) of the theorem, do not depend on $E(i)$.

The PQT makes three assertions:

(a) *Integer PQT*: If during the control parameters evolution no degeneracy of potential barriers can occur simultaneously with the minimal well depth degeneracy, then in the adiabatic followed by the low temperature ($T \to 0$) limits, the average number of system transitions through any link of a graph per cycle in the control parameters space is an integer.

(b) *Fractional PQT*: If we assume presence of permanent (rigid) degeneracy, so that some well depths or/and some potential barriers are identical during the whole cycle, then in the same limit the particle makes on average rational number of transitions through any link of a graph per cycle.

(c) *Strong PQT*: The quantization in (i) and (ii) is robust with respect to infinitesimal variations of the contour in the space of control parameters that does not violate the assumptions of (a) or (b). Remarkably, the opposite is also true: Robust operations of a molecular motor admit values in integer or rational numbers, respectively.

Theoretical results [2-5] provide the analytical/numerical approach to quantify sensitivity of a molecular motor to application of a periodic control signal and they suggest strategies for efficient molecular motor design.

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