A general discretization method for connecting free-energy landscape models of biomolecular motors to motor behaviour

P.T.T. Nguyen,[1,2] K.J. Challis[2] and M.W. Jack,[1] [1]Department of Physics, University of Otago, P.O. Box 56, Dunedin 9054, New Zealand and [2]Scion, Private Bag 3020, Rotorua 3046, New Zealand.

Biological systems use molecular motors to efficiently transform chemical energy into mechanical work. Biomolecular motors operate in cycles, far from equilibrium, and in an isothermal environment. Due to their small size, they are also significantly influenced by thermal fluctuations. To capture these general features of operation, we describe a molecular motor in terms of Brownian motion on a periodic free-energy landscape. This treatment is formulated in terms of a continuous diffusion equation for the probability density of the system. We develop a general discretization method that transforms the continuous diffusion equation to a discrete master equation. The resulting master equation is significantly simpler for calculating measurable properties of biomolecular motors and provides an opportunity to connect characteristics of the free-energy landscape with motor behaviour. We apply the method to a range of free-energy landscapes to explore motor behaviour in different regimes of operation.