QUANTUM CORRELATIONS IN COOPERATIVE TUNNELLING PROCESSES FOR A MODEL OF BIOLOGICAL ION CHANNELS

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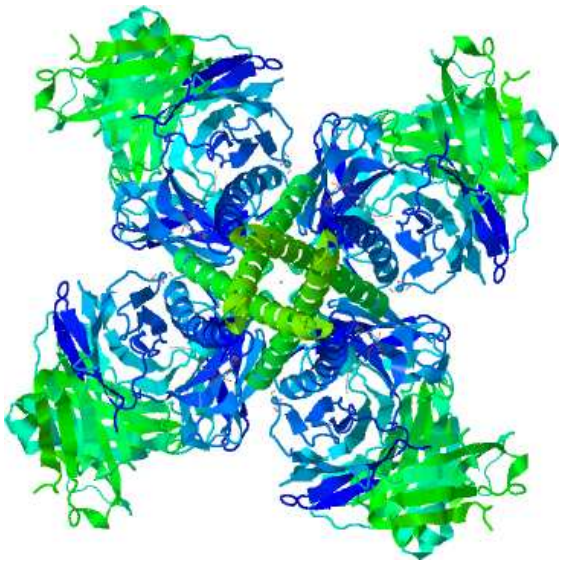
Outline

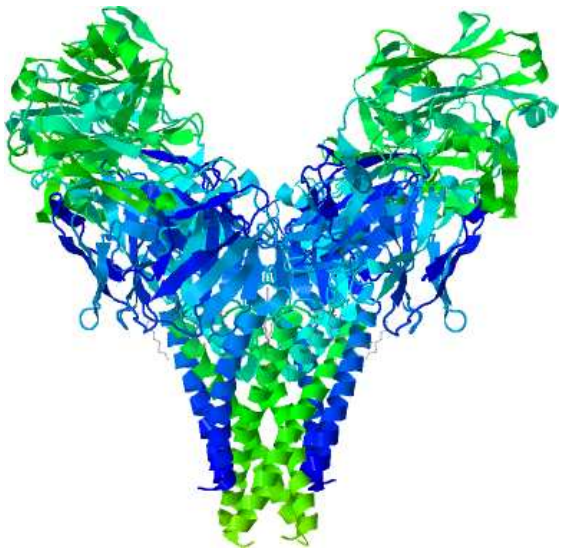
Motivation for Research

- Ion channels dictate charge transfer through cell membranes.
- Channels contain a small number of ions at any one time.
- Selecivity to particular ions.
- Diameter of channel is comparable to the size of an ion.

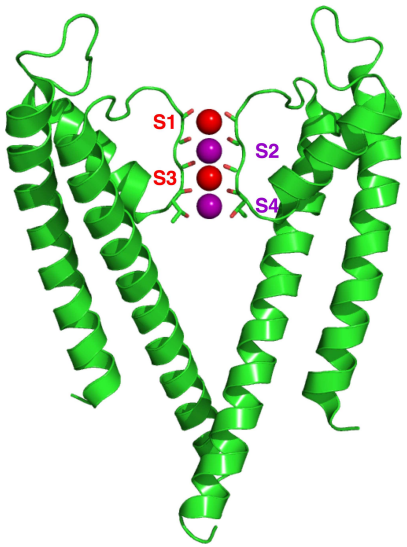
Selectivity Filter



(a) Plan view



(b) Cross-sectional view

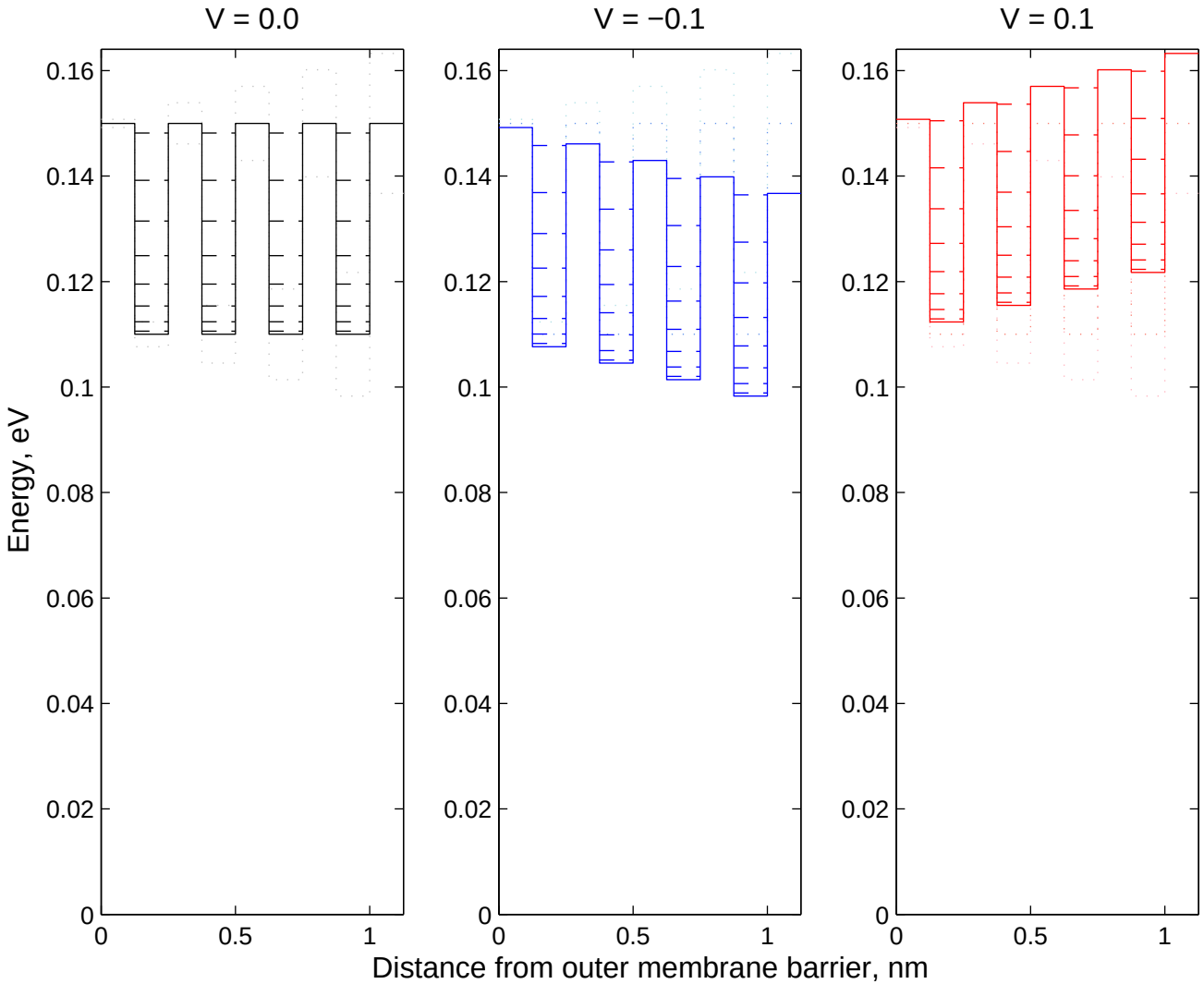


(c) Selectivity filter

- Four binding sites within selectivity filter [1].
- Model as square potential wells of equal depth at $V = 0$.

[1] Images of a potassium ion channel from PRB:1K4C

Model of selectivity filter



1. Coherent evolution between adjacent binding sites.
2. Incoherent jumps into, and out of particle reservoirs.
3. Radiative decay to lower discrete energy levels within potential well.
4. Non-radiative decay (mainly thermal dissipation) to an energetic equilibrium at finite temperature.
5. Dephasing
6. Thermal hopping between sites

Unconditional master equation

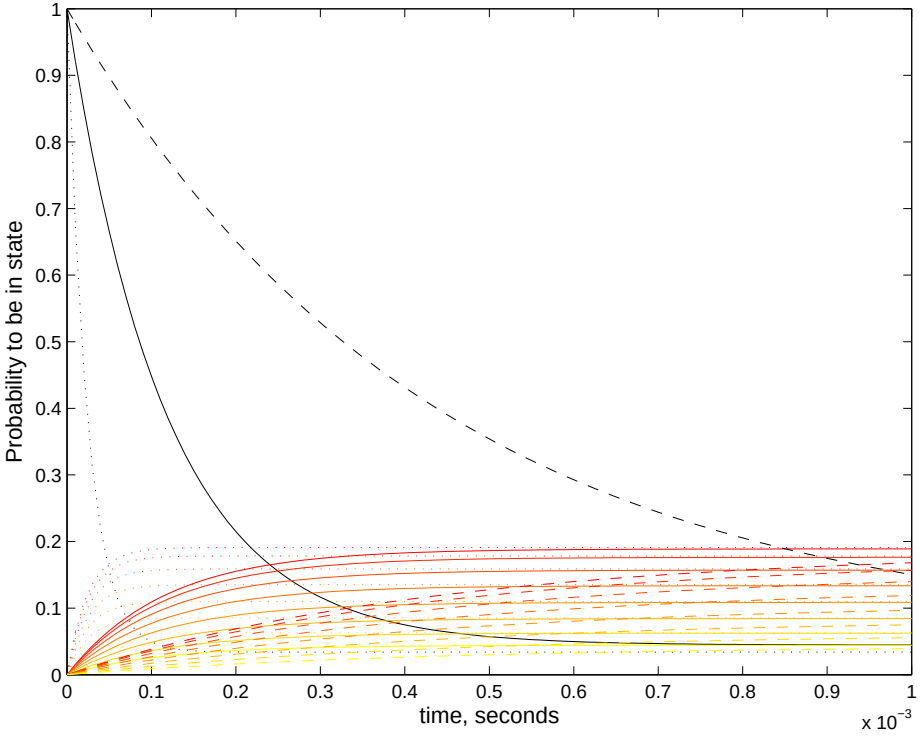
$$\frac{d\rho}{dt} = \frac{1}{i\hbar}\left[\hat{H},\rho\right] + \sum_{r=L,R} \Gamma\mathcal{D}[\hat{\sigma}_r]\rho + \Gamma\mathcal{D}[\hat{\sigma}_r^\dagger]\rho + \sum_w (\bar{n}+1)\gamma\mathcal{D}[\hat{a}_w]\rho + \bar{n}\gamma\mathcal{D}[\hat{a}_w^\dagger]\rho$$

$$\bar{n} = \frac{1}{exp\left(\frac{\hbar\omega}{K_B T}\right) - 1}$$

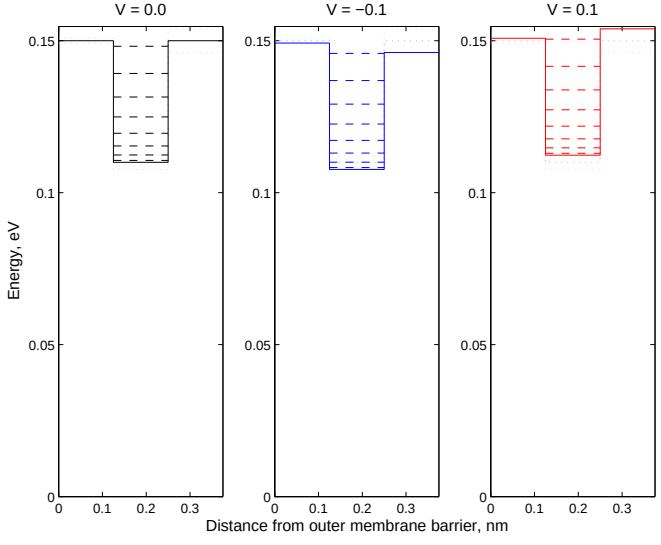
Stochastic evolution

- Uncondition master equation is useful to find analytic solution for small systems.
- Use stochastic evolution for larger systems.
- Point processes characterise quantum jumps.
- Hamiltonian evolution for coherent character.

Single well test, for ions

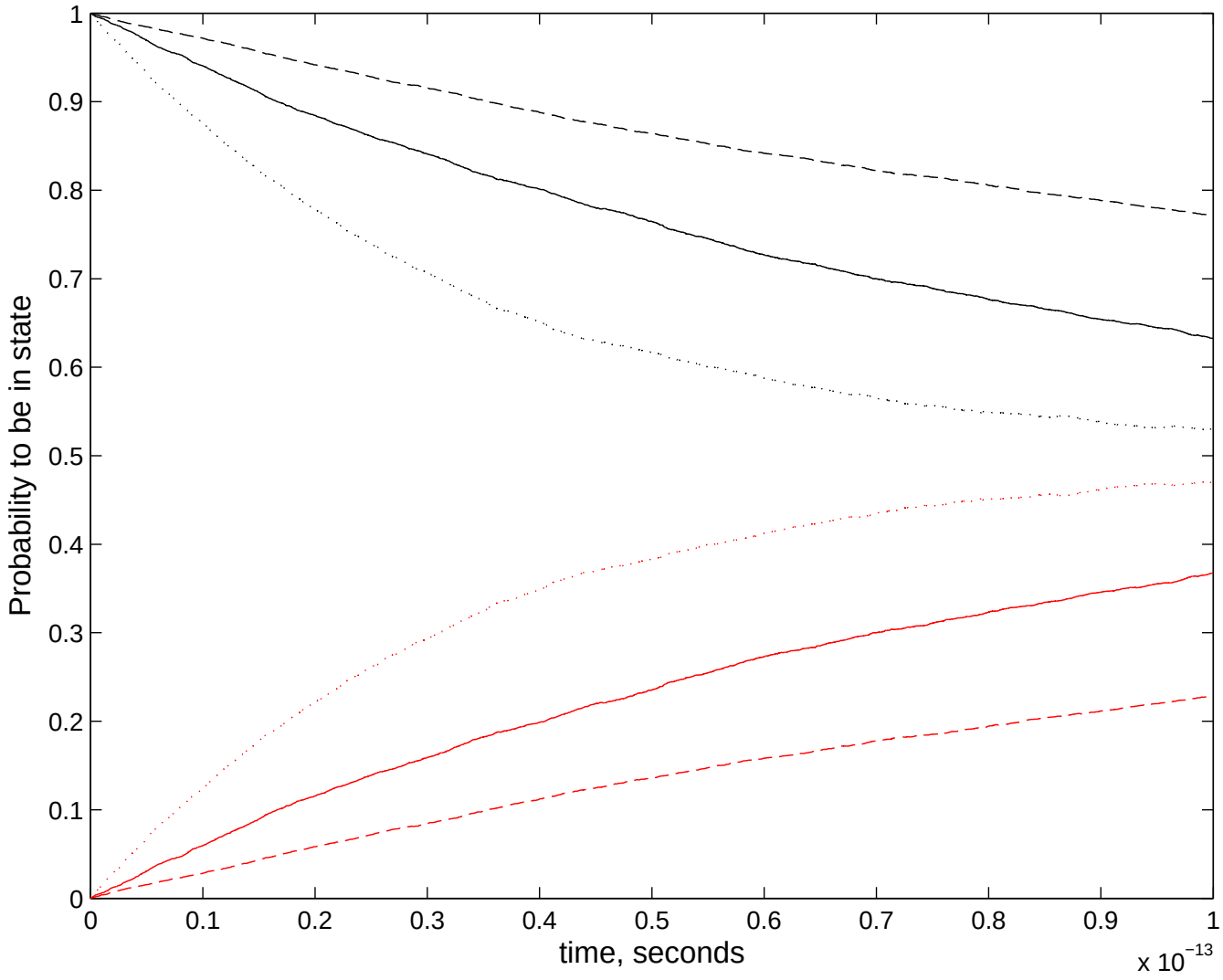


(d) Analytic solution to master equation of incoherent jumps. Colour scale, red to yellow, lower to higher energy levels, black is vaccuum state. Solid line V=0, dotted line V=-0.1, dashed line V=+0.1.

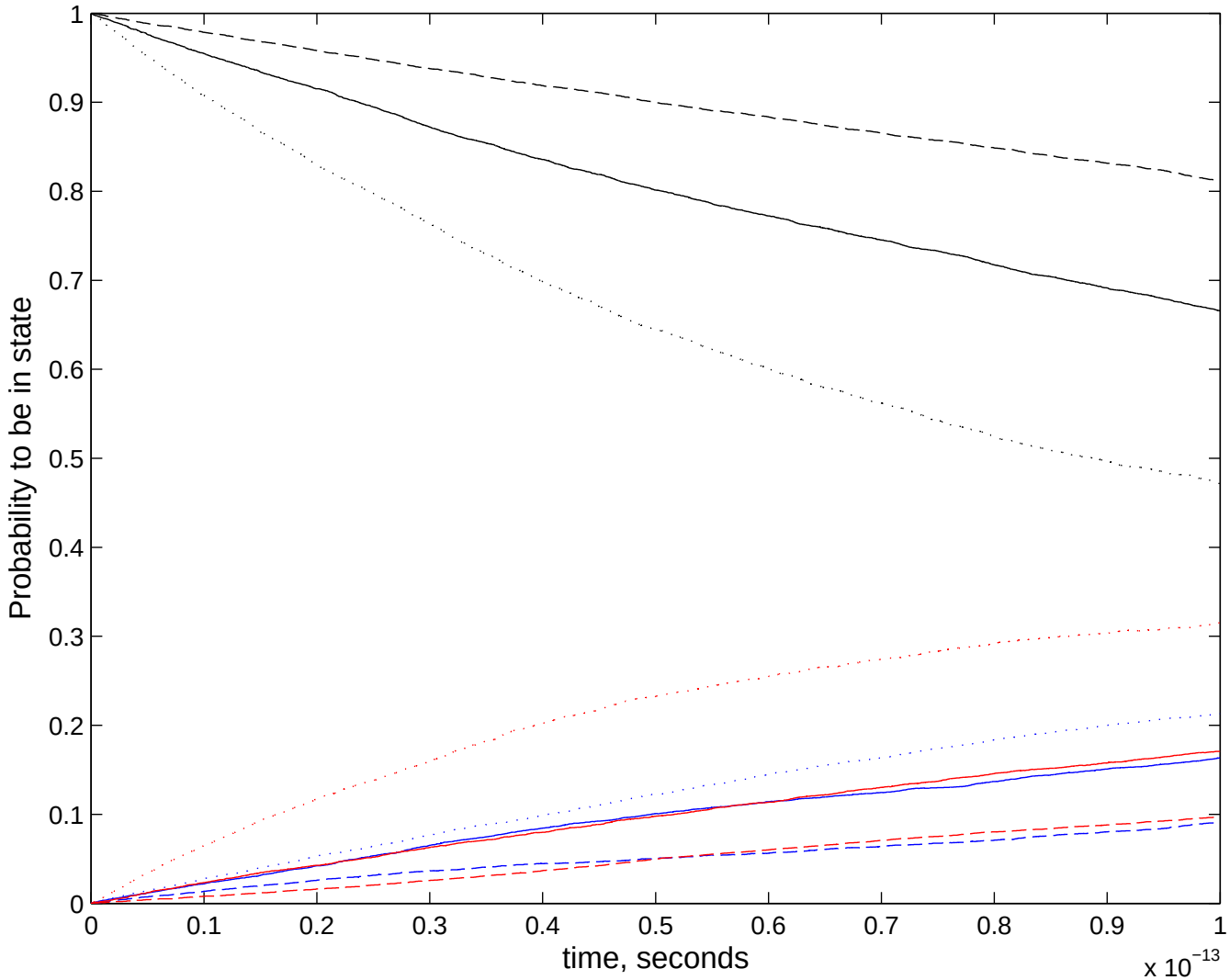


(e) Geometry and potential landscape of system

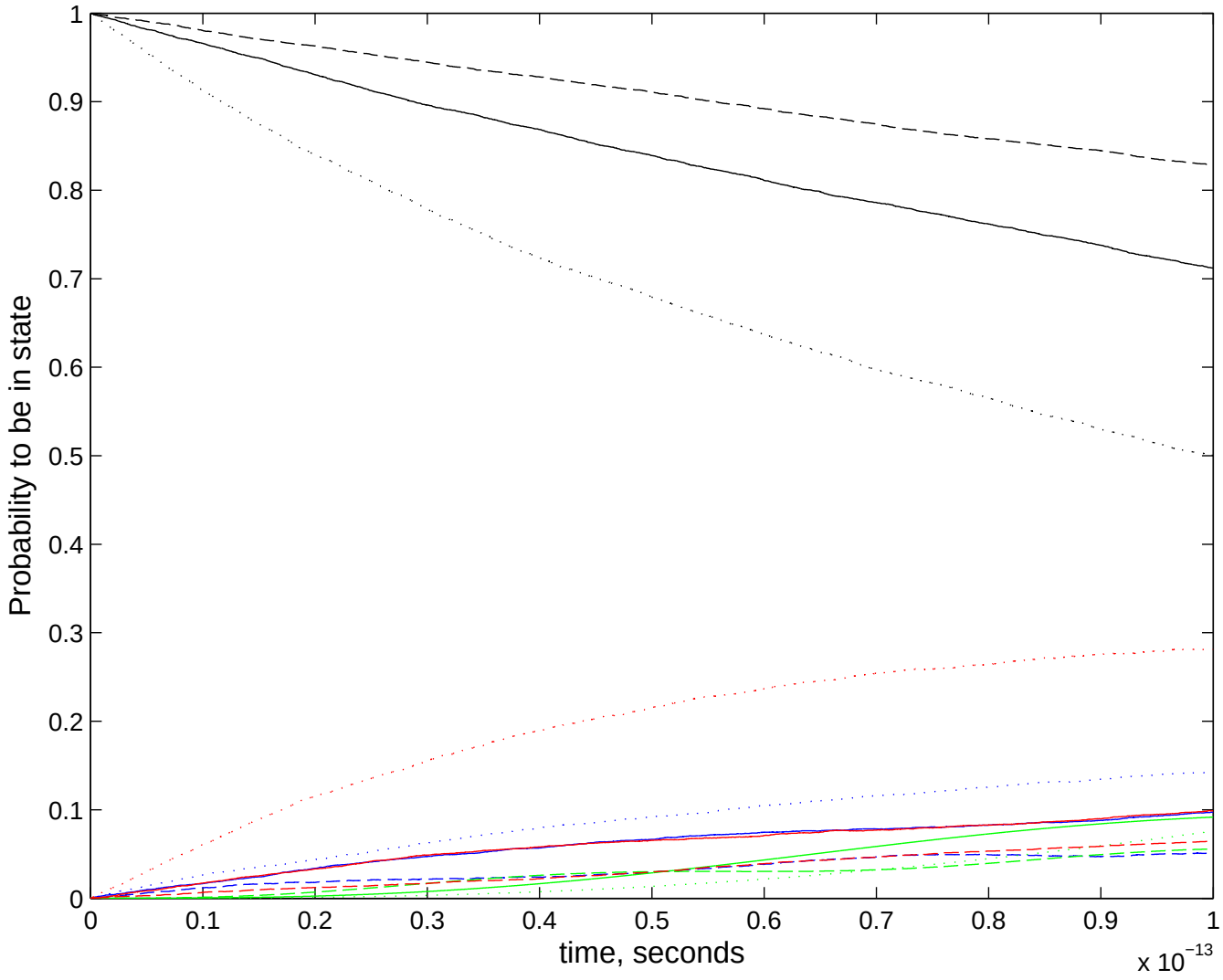
Single well, with two energy levels



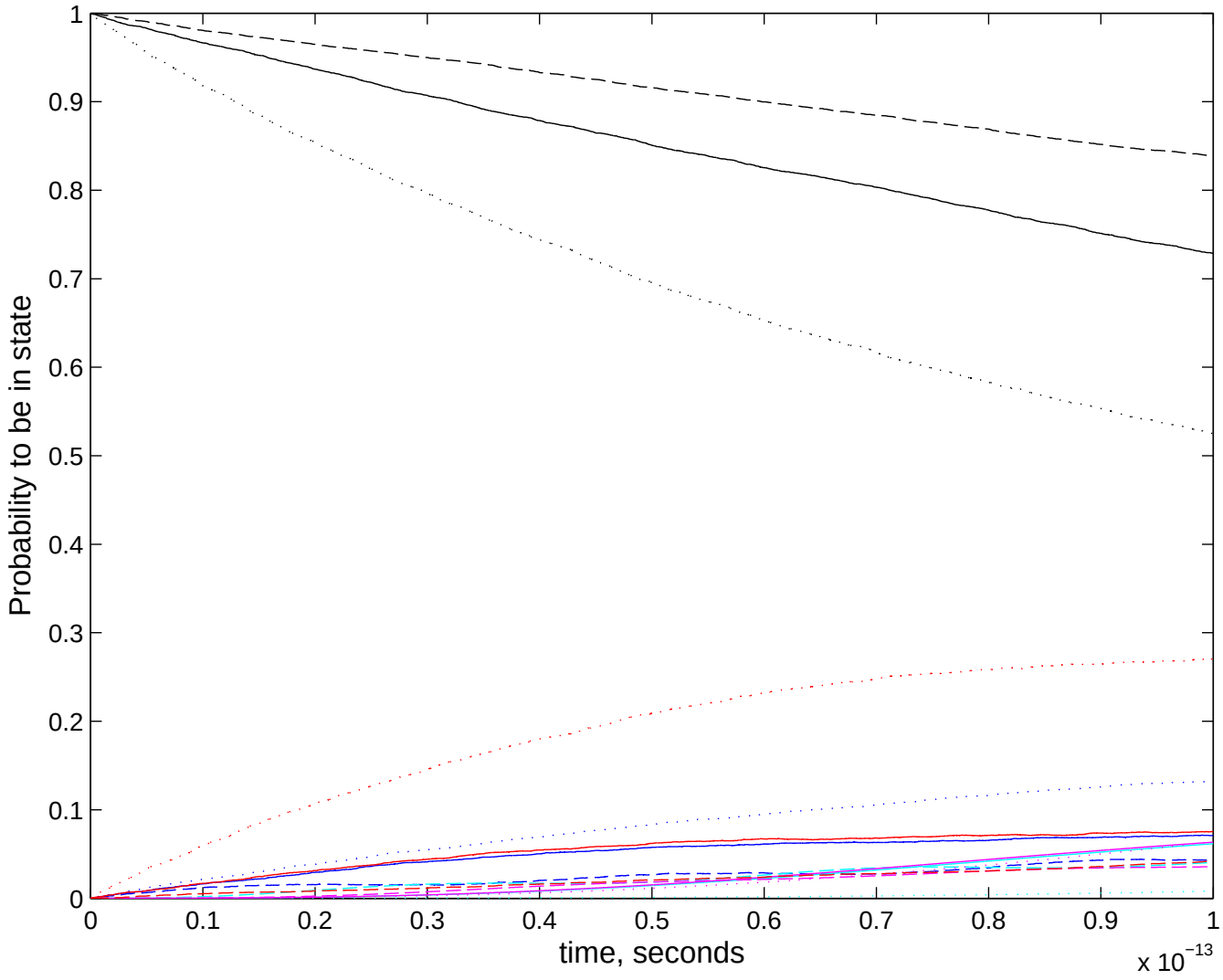
Two symmetric wells, each with two levels



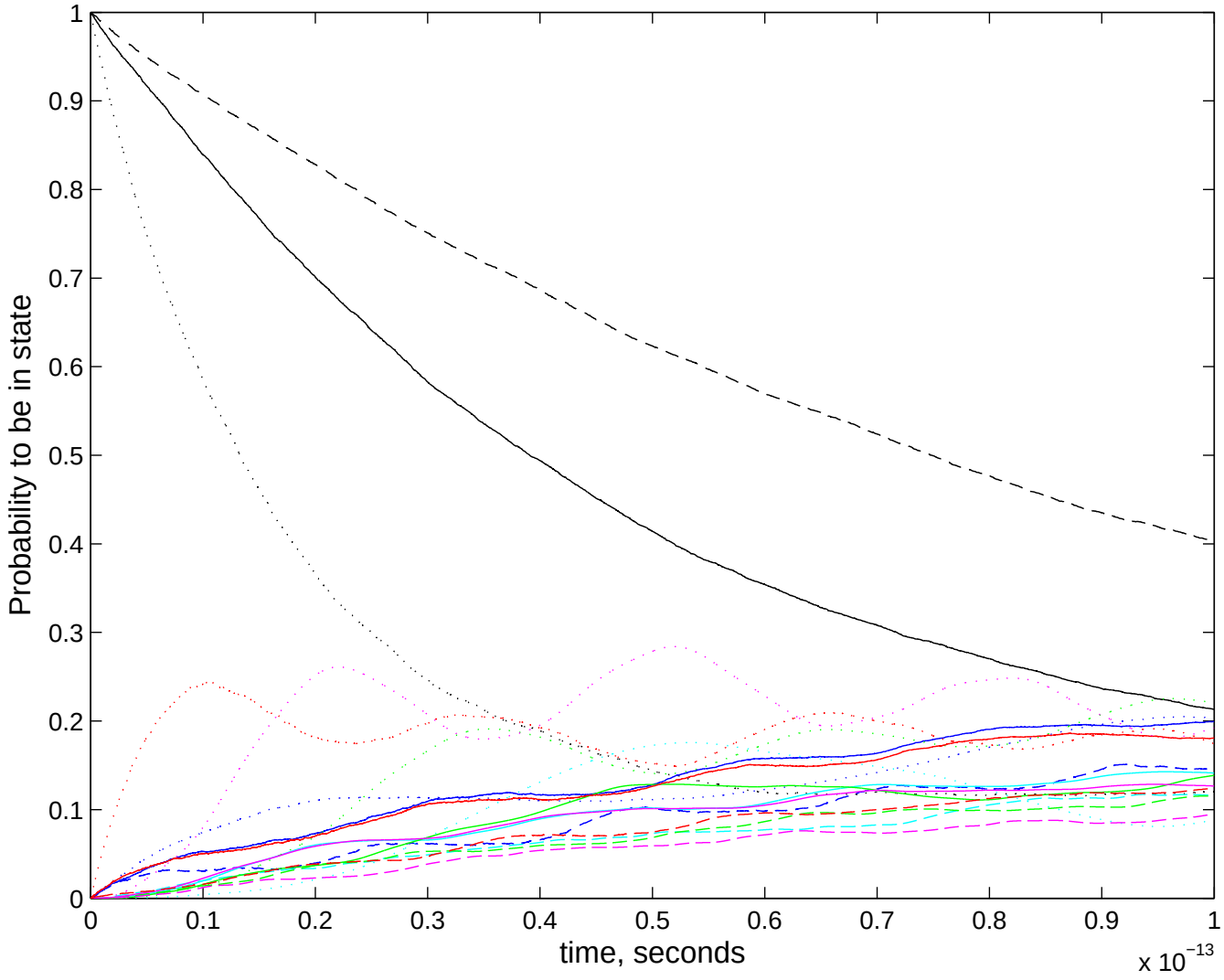
Three symmetric wells, each with two levels



Four symmetric wells, each with two levels



Four symmetric wells with an additional asymmetric well



Working to find quantum character for ion channels

1. Stochastically evolve ion channel system for selectivity filter.
2. Add cavity to selectivity filter.
3. Model a conical, extra-cellular region in additon to reservoir.
4. Allow 2 to 3 partices in the system at once.
5. Take account particle indistinguishability.