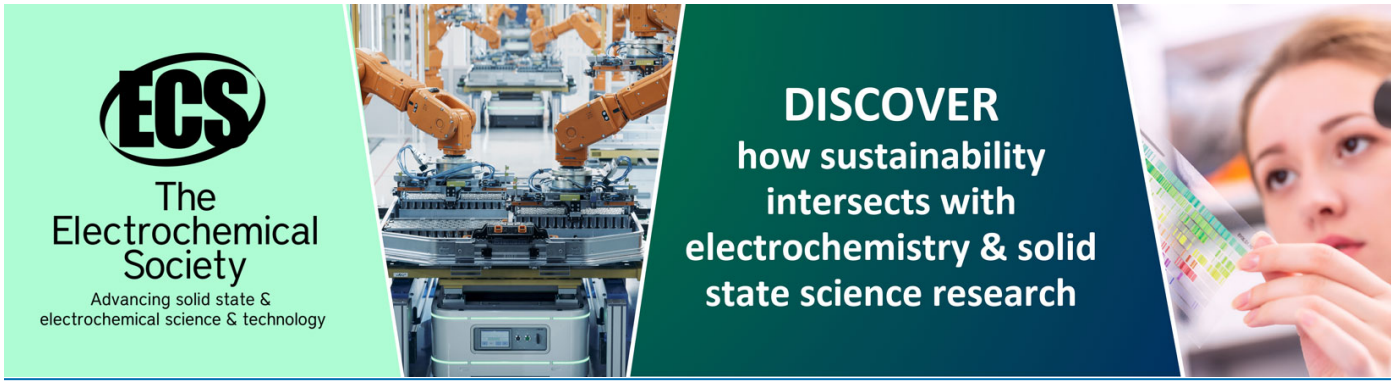
From Maximal Entropy Random Walk to quantum thermodynamics



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From Maximal Entropy Random Walk to quantum thermodynamics

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Abstract. Surprisingly, the natural looking random walk leading to Brownian motion occurs to be often biased in a very subtle way: emphasizing some possibilities by only approximating maximal uncertainty principle. A new philosophy of stochastic modelling has been recently introduced, in which we use the only maximizing entropy choice of transition probabilities instead. Local behaviour of both approaches is similar, but they usually lead to completely different global situations. In contrast to Brownian motion leading to nearly uniform stationary density, this recent approach turns out in agreement with having strong localization properties, thermodynamical predictions of quantum mechanics, like thermalizing to dynamical equilibrium state of probability density as the quantum ground state: squares of coordinates of the lowest energy eigenvector of the Bose-Hubbard Hamiltonian for single particle in discrete case, or of the standard Schrödinger operator while including potential and making infinitesimal limit.

While constructing probabilistic models, the choice of probabilities is often made arbitrarily. However, universal maximum uncertainty principle strictly imposes the optimal choice of probabilities as maximizing entropy for the knowledge we posses. For example, if among 2^n length n sequences of 0/1, we restrict to sequences in which $p \in [0,1]$ of symbols are "1", their number is approximately $\binom{n}{pn} \approx 2^{nh(p)}$, where $h(p) := -p\lg(p) - (1-p)\lg(1-p)$ is Shannon's entropy, which has single maximum for $p = 0.5$. The entropy is coefficient in the exponent, so in $n \to \infty$ limit, the maximizing entropy cases completely dominates all possibilities - without additional relations, a long random 0/1 sequence almost surely contains nearly half of "1" symbols.

Random walk is natural situation in physics of choosing probabilities - we discretize the space of possibilities and assume that because of complexity or our lack of information, the system makes transitions between these chosen states in practically random way. According to maximum uncertainty principle, as long as there are no additional clues about the transition probabilities, there should be used the maximizing entropy choice. The space of possibilities for any other choice becomes asymptotically negligible.

Specifically, for given graph defined by its adjacency matrix ($M_{ij} \in \{0,1\}$), we would like to choose transition probabilities ($0 \leq S_{ij} \leq M_{ij}$, $\sum_j S_{ij} = 1$), such that average entropy production ($H(S)$) is the largest possible: $H(S) := -\sum_i \pi_i \sum_j S_{ij} \lg(S_{ij})$, where $\pi_i \in [0,1]$ is stationary probability distribution for given S: $\sum_i \pi_i S_{ij} = \pi_j$, $\sum_i \pi_i = 1$. The standard choice leading to Brownian motion is that for each vertex, each outgoing edge is equally probable ($S_{ij}^{\mathrm{GRW}} = 1/\sum_j M_{ij} \;\Rightarrow\; \pi_i^{\mathrm{GRW}} \propto \sum_j M_{ij}$) - we will call such choice a Generic Random Walk. It can be seen as local approximation of entropy maximization. However, it usually is not

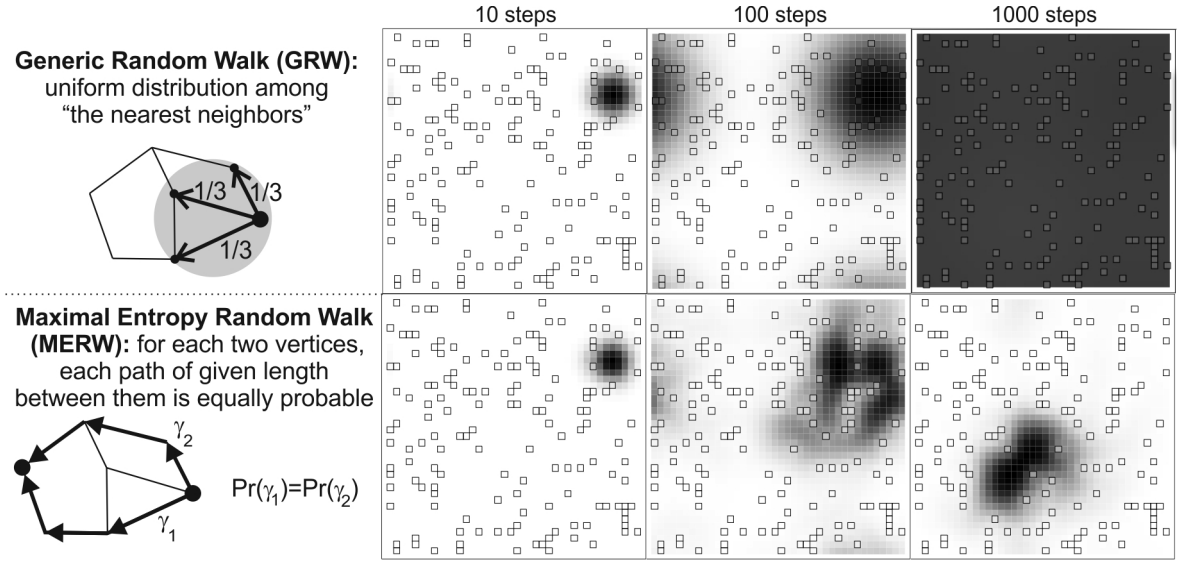

Figure 1. Schematic explanation of GRW and MERW choice of transition probabilities and simulation of their probability distribution evolution on 40×40 lattice graph with cyclic boundary conditions, in which all vertices but marked ones have self-loops (edge to itself).

the real maximum, which can be obtained by taking scale-invariant limit of GRW: instead of choosing uniform distribution among possible length 1 path, assume uniform probability among length k paths and take $k \to \infty$ limit. Such Maximum Entropy Random Walk is given by

$$S_{ij}^{\mathrm{MERW}} = \frac{M_{ij}}{\lambda}\frac{\varphi_j}{\varphi_i} \qquad \pi_i^{\mathrm{MERW}} \propto \varphi_i^2 \qquad \text{where} \qquad \sum_j M_{ij}\varphi_j = \lambda\varphi_i$$

is the dominant eigenvector. Local behaviour of both GRW and MERW looks similar, but from Fig. 1 we see that on defected lattice they lead to completely different stationary distributions - GRW to nearly uniform one, while MERW has strong localization properties ([1], [2]) - in this case practically completely localizes in the largest defect-free region (called Lifshitz sphere).

The adjacency matrix can be seen as minus Hamiltonian of Bose-Hubbard model for single particle - the dominant eigenvector corresponds to quantum ground state and so in opposite to GRW, MERW stationary probability distribution agrees with thermodynamical prediction of quantum mechanics: deexcitation to the ground state density. This localization effect can be seen in recent STM measurements of electron density on defected lattice of semiconductor [3].

The defects from Fig. 1 can be seen as locally larger potential - after generalization into continuous potential and taking infinitesimal limit of such lattice, the Hamiltonian becomes Schrödinger operator. It also leads to thermodynamical analogues of Ehrenfest equation, Heisenberg uncertainty principle and Pauli exclusion principle [4].

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