# From traffic jams on RNA to the quantum mechanics of spin chains.

1. **Kinetics of biopolymerization on nucleic acid templates.**
Authors: C. T. MacDonald, J. H. Gibbs and A. C. Pipkin
Biopolymers, 6(1), pp.1-25 (1968)

2. **Bethe solution for the dynamical-scaling exponent of the noisy Burgers equation.**
Authors: Leh-Hun Gwa and Herbert Spohn
Phys. Rev. A 46, 844 (1992)

3. **Exactly Solvable Models for Many-Body Systems Far from Equilibrium.**
Authors: G. M. Schütz and K.J. Wiese
Vol.19, Phase Transitions and Critical Phenomena, edited by Domb and Green (2001)

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It is not so very often that molecular biology inspires an interesting application of quantum many-body physics. However in the first of the three recommended papers, Macdonald et al. proposed in 1968 a simple mathematical model for protein synthesis that (eventually) had just such an effect. Proteins are synthesized by ribosomes using messenger RNA (mRNA) gene transcription strands as templates. In this process, ribosomes attach themselves to the transcripts as they emerge from RNA polymerase enzymes "walking" along a DNA genome molecule. A ribosome attaches itself to a start site on the mRNA strand and then moves from RNA base to RNA base while synthesizing a string of peptides (amino-acids). Triplets of RNA bases correspond to particular amino-acids. When a ribosome reaches a stop site at the end of the mRNA strand, it leaves. The resulting polypeptide string folds into a protein. Electron microscopy reveals that, during active gene transcription, each mRNA strand is quite crowded with ribosomes. It might seem that maximum ribosome occupancy should produce the maximum protein synthesis rate but this is not so obvious. It is well-known to the citizens of Los Angeles that densely packed freeways often have levels of traffic flow close to zero. In the opposite limit, with few cars on the road, each car can drive at (or more likely above) the speed limit but the total traffic flow still is low. Evidently, there is some intermediate density that maximizes the flow. This feature is demonstrated by the model of Macdonald et al.

Assume a chain of $L$ adjacent cells that can contain particles. A cell contains either zero or one particle. Particles are inserted in the first cell at a rate $\alpha$ and removed from the last cell at a rate $\beta$. At every time step, particles either hop to an unoccupied cell on the right with probability $p$ or to an unoccupied cell on left with probability $q = 1 - p$. This non-equilibrium stochastic Markov process is the "Asymmetric Exclusion Process" (ASEP) with the $p = 1$ case known as the TASEP model (T stands for "totally"). The ASEP model is an example of a *driven* Markov process that does not evolve to a steady-state that obeys detailed balance and for which there is no equivalent of a Boltzmann distribution.

Steady-state solutions have been found for the ASEP process. The particle density $\rho$ that optimizes the current for the ASEP model would be expected to be $\rho = 1/2$ since this allows for the possibility that the particles march collectively one step to the right for every time unit (though in actuality the process remains stochastic). More generally, the current density can be shown to be $j(\rho) = \rho(1 - \rho)$. In an $\alpha - \beta$ diagram the three steady-state solution (congested high-density, speed limit low-density, and maximal current) are separated from each other by boundary lines that mark mathematical singularities (in the $L \to \infty$ limit). It is surprising to encounter the equivalent of a phase-transition in a one-dimensional many-body system with short-range interactions and it is also surprising that the state of the system is determined by *boundary conditions.*

The continuum limit of the ASEP model is found by noting that at low densities $\rho$ the ASEP particles must perform a (biased) random walk. This can be accounted for by adding the noisy diffusion current $-D\frac{\partial \rho}{\partial x} - \eta(x,t)$ to $j(\rho)$ with $D$ the diffusion coefficient of the random walk and $\eta(x,t)$ a noise source. This leads to the *noisy Burgers equation*:

$$\frac{\partial \rho}{\partial t} + \frac{\partial j(\rho)}{\partial x} = \frac{\partial}{\partial x}\left(D\frac{\partial \rho}{\partial x} + \eta(x,t)\right). \tag{1}$$

The Burgers equation, which can be viewed as a one-dimensional version of the Navier-Stokes equation with viscosity $D$, has solutions corresponding to propagating shock waves that gradually dissipate away (another familiar feature of freeway traffic). This suggests that the steady-state solutions could have excitations corresponding to traveling shock waves.

The second of the recommended papers, by Gwa and Spohn, is a mathematical tour de force that provides us with the spectrum of excitations. First, they relate the ASEP to a quantum many-body problem, specifically a version of the one-dimensional spin 1/2 XXZ Heisenberg model:

$$H = \sum_{i=1}^{L}\left(p\sigma_i^- \sigma_{i+1}^+ + q\sigma_i^+ \sigma_{i+1}^- + \frac{1}{4}\sigma_i^z \sigma_{i+1}^z\right) \tag{2}$$

constructed from the usual spin 1/2 Pauli spin matrices. This version of the Heisenberg spin chain has an odd feature: unless $p = q = 1/2$, $H$ is *non-Hermitian.* One of the consequences is that the eigenvalues of this Hamiltonian need not be real numbers. Recall that for conventional quantum mechanics, observable quantities are represented by Hermitian operators with real eigenvalues.

Gwa and Spohn then use the *Bethe Ansatz* to obtain excitation energies for the ASEP. In the Bethe Ansatz, many-body wavefunctions are constructed as a linear superposition of plane wave states, permuting momenta and coordinates. The lowest excited state has an energy eigenvalue $E_1$ given by

$$E_1 = -2\sqrt{\rho(1-\rho)}\frac{6.51..}{L^{3/2}} \pm 2\pi i \frac{2\rho - 1}{L} \tag{3}$$

As advertised, it is a complex number. The physical meaning of $E_1$ is that the lowest excited state has a time dependence proportional to $\exp E_1 t$. The relaxation rate of the many-body system thus has a power-law dependence on system size $L$. If we equate $1/L$ with a wavevector $k$ then this correspond to a dynamical critical exponent $z = 3/2$, consistent with the KPZ model. The imaginary part of the eigenvalue indicates that the excitation is a propagating wave.

The paper by Gwa and Spohn is too dense for a first encounter with ASEP. The third of the recommended papers is an outstanding review article by Schütz and Wiese provides the reader with a careful introduction to solution methods not just for ASEP but also for other non-equilibrium many-particle systems. They clearly explain the general connection between quantum statistcal physics with non-Hermitian Hamiltonians and Markov processes. Let $P_\eta(t)$ be the time-dependent probability distribution for a microstate $\eta$. For example for ASEP, one can denote microstates by the $L$ component vectors $|\eta\rangle$ of ones and zeros depending on whether or not a cell is occupied. The state of a system is defined by the probability vector $|P(t)\rangle = \sum_\eta P_\eta(t)|\eta\rangle$. Let $w_{\eta|\eta'}$ represent the transition rate from state $\eta$ to state $\eta'$. For a Markov process, the probability distribution $P_\eta(t)$ obeys the Master Equation

$$\frac{dP_\eta(t)}{dt} = \sum_{\eta' \neq \eta} \left[ w_{\eta'|\eta} P_{\eta'}(t) - w_{\eta|\eta'} P_\eta(t) \right] \tag{4}$$

In vector notation, the master equation can be expressed as

$$\frac{d}{dt}|P\rangle = H|P\rangle \tag{5}$$

The off-diagonal entries of the matrix $H_{\eta|\eta'}$ equal $w_{\eta|\eta'}$ while the diagonal entries $H_{\eta|\eta}$ equal $-\sum_{\eta' \neq \eta} w_{\eta'|\eta}$. After analytical continuation to imaginary time, this equation reduces to the Hamiltonian matrix form of quantum mechanics. For asymmetric exclusion processes $w_{\eta|\eta'} \neq w_{\eta'|\eta}$. In this case, the Hamiltonian is a real, asymmetric matrix and thus non-Hermitian.

This mapping from a non-equilibrium classical stochastic many-body problem onto a quantum many-body problem is interesting in its own right but the real "pay-off" comes when the a mapping allows the application of a powerful method of quantum mechanics, such as the Bethe Ansatz. One might imagine working backwards. If one knows of a solvable quantum many-body problem, such as the Kondo problem, is there perhaps an interesting classical stochastic problem that corresponds to that? There is currently great interest in driven systems far from thermodynamic equilibrium, in particular in the context of the "fluctuation theorems". The ASEP case is a rare example of a model for which exact results can be been obtained. It has a number of interesting features that encourage further study. However, the solution method we discussed "works" only in one dimension. The current situation for the statistical physics of driven systems resembles that of the 1930's when only one-dimensional statistical mechanics problems were soluble. What is needed is an Onsager who can extend these methods to higher dimensions!