Stochastic reaction-diffusion processes may be presented in terms of integrable quantum chains and can be used to describe various biological and chemical systems. Exploiting the integrability of the models one finds in some cases good agreement between experimental and exact theoretical data. This is shown for the Rubinstein-Duke model for gel-electrophoresis of DNA, the asymmetric exclusion process as a model for the kinetics of biopolymerization and the coagulation-diffusion model for exciton dynamics on TMMC chains.

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1 Introduction

It has been realized in recent years that the stochastic time evolution of many one-dimensional reaction-diffusion processes can be mapped to integrable quantum chains. This insight has made available the tool box of integrable models for these interacting particle systems far from equilibrium and has led to many new exact results for their dynamical and stationary properties. It is also amusing to note that the Hamiltonians for such systems are, in general, not hermitian and therefore from a quantum mechanical point of view not interesting. The interpretation as time evolution operators for stochastic dynamics thus extends the physical relevance of integrable systems to non-hermitian models.

The relationship between stochastic dynamics and quantum chains is conceptually very simple: At any given time $t$ the state of the system is completely described by a probability distribution $f(n; t)$ for the stochastic variables $n$. The time evolution of this distribution is governed by a master equation which expresses the probability of finding the system at time $t + dt$ in a given configuration in terms of the probability distribution at time $t$ through a first order differential equation in the time variable. Such a master equation can be expressed in a “quantum Hamiltonian formalism” by mapping each state of the system to a basis vector in a suitable vector space $\mathcal{X}$. In this mapping the probability distribution at time $t$ becomes a vector $\left| f(t) \right>$ and the master equation takes the form

$$\frac{d}{dt} \left| f(t) \right> = -H \left| f(t) \right>$$

(1)

where $H$ is a suitably chosen linear map acting on $\mathcal{X}$. For many systems of interest, $H$ is the Hamiltonian of some integrable quantum chain.\(^2\)

A severe constraint to the application of such models to experiments seems to be the fact that they are all one-dimensional. However, it turns out that for many situations e.g. involving polymers or traffic models, a one-dimensional description of the stochastic dynamics is appropriate. Furthermore there are systems where only the projection of the system onto one space coordinate is of actual experimental interest. In these cases integrable reaction-diffusion processes can and do play a role.

\(^2\)See e.g. the paper on Stochastic Reaction-Diffusion Processes, Operator Algebras and Integrable Quantum Spin Chains in this volume and references therein.
Here we will briefly review three different systems where integrable models are of experimental relevance: Firstly the Rubinstein-Duke model for the description of gel-electrophoresis of DNA (Sec. 2), then the asymmetric exclusion process with open boundary conditions for the kinetics of biopolymerization on nucleic acid templates (Sec. 3) and the one-species coagulation-diffusion model for exciton dynamics on laser excited TMMC chains (Sec. 4).

2 Gel-Electrophoresis of DNA

A widely used and simple method for the separation of DNA fragments of different length is DC gel-electrophoresis. The DNA mixture to be separated is introduced into a gel matrix. Since the DNA is charged, it will move in a constant electric field $E$ with velocity $v(E, N)$ where $N$ is the length of the fragment. After some time fragments of different length will have travelled a distance in the gel depending on their length and can therefore be separated. Clearly it would be desirable to have a quantitative understanding of the motion of DNA in gels.

Based on the earlier concepts of the confining tube[1] and of reptation[2] Rubinstein[3] and Duke[4] introduced a simple model for the motion of a polymer in a gel matrix. In this model the gel is idealized by a regular cubic lattice where the cells are the pores of the gel through which the polymer reptates. The polymer itself is represented by a string of reptons, the number of which is the length of the polymer divided by its persistence length. These reptons hop stochastically from pore to pore according to rules based on the mechanism of reptation and assuming local detailed balance. Since in electrophoresis only the average velocity of the center of mass in field direction is of interest, one can project the motion of the reptons onto this direction. Some mappings that we will not describe here lead finally to a lattice gas model representing the relative motion of all reptons in field direction. The motion perpendicular to the field is diffusive with a diffusion constant[3,4] $D = 1/3N^2$ entering the drift velocity $v(E, N)$ for small $E$ through the Nernst-Einstein relation[3,4] $v = DNE$.

Here we will not give the details of the mapping to the lattice gas model but just state the resulting lattice gas dynamics[4]. There are two kinds of particles, $A$ and $B$, moving on a lattice of $L = N - 1$ sites and each site can occupied by at most one particle, $A$ or $B$. $A$-particles hop to right
(left) with rate \( q \) \((q^{-1})\) if the site is unoccupied. Here \( \ln(q) \) is the energy gain when a repton moves into a pore in field direction. On site 1 of the chain \( A \)-particles are created (annihilated) with rate \( q \) \((q^{-1})\), while on site \( L \) they are annihilated (created) with rate \( q \) \((q^{-1})\). For the \( B \)-particles the same rules hold, but with \( q \) and \( q^{-1} \) interchanged. It is easy to show that the average drift velocity \( v(E,N) \) is the difference between the stationary current \( J_A(E,N) - J_B(E,N) \) of \( A \) particles and \( B \) particles.

The stationary distribution of the system is not known except in the periodic system\(^8\) which does not have an interpretation in terms of polymers moving through a gel. However, extensive Monte-Carlo studies\(^9\) have provided a good and reliable knowledge of \( v \) in the framework of the model. The surprise is that these results are in excellent agreement with experimental data\(^10, 11\). This gives confidence that despite all its simplifications, the Rubinstein-Duke model captures the essential physical processes involved and allows for reliable predictions in real gel-electrophoresis.

In order to make contact with integrable models we write the master equation of the process in the quantum Hamiltonian formalism. The stochastic time evolution of the system is given by the Hamiltonian of a three-states quantum chain\(^\text{\textsuperscript{11}}\)

\[
H(\alpha, q) = b_1(\alpha, q) + b_L(\alpha, q^{-1}) + \sum_{i=1}^{L-1} u_i(q)
\]  

(2)

where \( b_i(\alpha, q) = \alpha q(1 - n_i^A - a_i^- - b_i^-) + \alpha q^{-1}(1 - n_i^B - a_i - b_i^+ \) and \( u_i(q) = q(n_i^A n_{i+1}^0 + n_i^0 n_i^B - a_i a_i^+ - b_i^- b_{i+1}) + q^{-1}(n_i^A n_{i+1}^0 + n_i^0 n_i^B - a_i^+ a_i - b_i b_i^+ \). Here \( n_i^A \equiv E_{i1}^1 \), \( n_i^B \equiv E_i^{33} \) and \( n_i^0 \equiv 1 - n_i^A - n_i^B \equiv E_i^{22} \) are projection operators on states with an \( A \)-particle, vacancy and \( B \)-particle resp. on site \( i \). The operators \( a_i \equiv E_i^{21}, a_i^+ \equiv E_i^{12}, b_i \equiv E_i^{23}, \) and \( b_i^+ \equiv E_i^{32} \) are annihilation and creation operators for \( A \)- and \( B \) particles. \( E_i^{jk} \) is the \(3 \times 3\) matrix with matrix elements \( (E_i^{jk})_{\alpha,\beta} = \delta_{j,\alpha}\delta_{k,\beta} \) acting on site \( i \). The factor \( \alpha \) takes into account the possibility of a different mobility of the end-reptons compared to those in the bulk.

Nothing is known about the integrability of the model in non-zero field. However, if no field is applied \((q = 1)\) and if the ends of the polymer are fixed in the gel \((\alpha = 0, \text{e.g. by making a chemical bond with an immobile particle})\), then \( H \) is integrable. In this case the model describes the internal random fluctuations of the polymer within the gel. That \( H(0,1) \) is integrable.
can be seen by verifying that for $\alpha = E = 0$ the Hamiltonian for both the isotropic spin-1/2 Heisenberg chain with open boundary conditions and the Rubinstein-Duke model have the form $H = \sum_{i=1}^{L-1} u_i$ where the $u_i$ satisfy the same Temperley-Lieb algebra $u_i^2 = 2u_i$, $u_iu_{i+\pm 1}u_i = u_i$, $[u_i, u_j] = 0$ for $|i - j| \geq 2$. Using the Bethe ansatz one can compute the relaxation of the DNA to equilibrium (where each configuration is equally probable).

If the ends of the polymer are not kept fixed, then the model has at least an integrable subspace with a spectrum which is identical to that of the isotropic Heisenberg chain with non-diagonal, symmetry breaking boundary fields. This can be shown by using a similarity transformation on $H$ and projecting on one of its invariant subspaces. In this case one can use the integrability to obtain the relaxation of the distribution of vacancies. This gives the density of reptons per pore in a freely diffusing polymer.

Remarkably the model predicts that there is no band collapse if one pulls only at one end of the polymer rather than at each repton with some external field. The velocity is then always length dependent and asymptotically given by the exact expressions $v = E/3N^2$ for $E \to 0$ and $v = 1/(3N - 5)$ for $E \to \infty$. In this case $H$ consists of the integrable zero-field bulk part and boundary terms $b_1(1, q) + b_L(1, 1)$. Whether this model is integrable is not clear and it would be interesting to ask generally which integrable boundary conditions one can obtain for the model with vanishing bulk field.

3 Kinetics of Biopolymerization

Back in 1968 MacDonald et al. studied the kinetics of biopolymerization on nucleic acid templates. The mechanism they try to describe is (in a very simplified manner) the following: Ribosomes attach to the beginning of a messenger-RNA chain and “read” the genetic information which is encoded in triplets of base pairs by moving along the m-RNA. At the same time the ribosome adds monomers to a biopolymer attached to it: Each time a unit of information is being read a monomer is added to a biopolymer attached to the ribosom and which is in this way synthesized by the ribosom. After having added the monomer the ribosom moves one triplet further and reads again. So in each reading step the biopolymer grows in length by one monomer. Which monomer is added depends on the genetic information.

\[\text{The m-RNA is a long molecule made up of such consecutive triplets.}\]
read by the ribosom. The ribosomes are much bigger than the triplets on the m-RNA, they cover 20-30 of such triplets. Therefore neighbouring ribosomes sitting at the same time on the m-RNA cannot simultaneously read the same information. Furthermore they cannot overtake each other: If a ribosom sits at a particular place on the m-RNA and does not (temporarily) proceed further (e.g. because no appropriate monomer has been found in the surrounding medium for the polymerization process), then an oncoming ribosom from behind will stop until the first has eventually moved on.

In order to describe the kinetics of this process MacDonald et al. introduced the following simple model. The m-RNA is represented by one-dimensional lattice of \( L \) sites where each lattice site represents one triplet of base pairs. The ribosom is a particle covering \( r \) neighbouring sites (for real systems \( r = 20 \ldots 30 \)) but moving by only one lattice site in each (infinitesimal) time step with a constant rate \( p \). These particles interact via hard-core repulsion, i.e. there is no long range interaction, but there is also no overlap of ribosomes. In principle one can also allow for back-hopping with a non-vanishing rate \( q \). At the beginning of the chain particles are added with rate \( \alpha p \) and at the end of the chain they are removed with rate \( \beta p \). Again, one may also allow for a removal rate \( \alpha' q \) at the beginning of the chain and an addition rate \( \beta' p \) at the end of the chain.

In the idealized case \( r = 1 \) this model became later known as the asymmetric exclusion process with open boundary conditions\(^{18}\). Its steady state was first studied using a mean-field approach\(^{16}\). Then in a following paper\(^{17}\) the generalized case \( r > 1 \) was studied numerically and compared to experimental data on the stationary density distribution of ribosomes along the chain. These were found to be consistent with the results obtained from the model with \( q = 0 \) and \( \alpha = \beta < p/2 \). Furthermore it turned out that the phase diagram for general \( r \) is similar to the much simpler case \( r = 1 \) in the sense that there are three distinct phases, a low density phase, a high density phase and a maximal current phase (see below). These observations encourage to use the asymmetric exclusion process as a simple but in certain aspects realistic model for this biological system.

The experimentally relevant case is the phase transition line from the low-density phase to the high density phase. On this phase transition line the mean-field and numerical calculations predict a region of low density of ribosomes from the beginning of the chain up to some point where the
density suddenly jumps (over a few lattice sites) to a high density value. In the maximal current phase \( \alpha, \beta > p/2 \) mean-field predicts a power law decay of the stationary density to a constant bulk value, \( \rho(x) - \rho_{\text{bulk}} \propto x^{-1} \), where \( x \) measures the distance from the ends of the chain. In this case the polymerization determines the profile rather the initialization and release rates \( \alpha, \beta \).

These predictions and the apparent experimental relevance of the model make an exact solution of at least the simple case \( r = 1 \) desirable. The stochastic dynamics of the model are given in the quantum Hamiltonian formalism by the integrable Hamiltonian of the anisotropic spin-1/2 Heisenberg chain with non-diagonal boundary fields:

\[
H = -\alpha p \left[ s_i^- - (1 - n_i) \right] - \beta p \left[ s_i^+ - n_i \right] - \sum_{i=1}^{L} \left[ p \left( s_i^+ s_{i+1}^- - n_i(1 - n_{i+1}) \right) + q \left( s_i^- s_{i+1}^+ - (1 - n_i)n_{i+1} \right) \right].
\] (3)

Here \( s_\pm = (\sigma^x \pm i\sigma^y)/2 \) and \( n = (1 - \sigma^z)/2 \). For \( \alpha = \beta = 0 \) this reduces to the \( SU(2)_q \) symmetric quantum chain with diagonal boundary fields which can be solved by the coordinate or algebraic Bethe ansatz. However, the boundary fields given here break the \( U(1) \) symmetry of the model and other approaches are necessary to find at least the steady state of the system, i.e. the ground state of \( H \) with (by construction) energy 0. In what follows we will consider only \( q = 0 \). We set \( p = 1 \) which is no loss in generality since it sets only the time scale of the process.

The breakthrough to the exact solution came only more than 20 years after the work on biopolymerization and independently of it.\textsuperscript{[19, 20, 21]} It turned out that the solution of the master equation of a system of \( L \) sites can be recursively expressed in terms of the solution for \( L - 1 \) sites\textsuperscript{[19]}. The exact solution obtained from the solution of these recursion relations reproduces the three phases predicted by mean field, but shows more structure inside the low- and high-density phases\textsuperscript{[20]}. This reveals an intricate interplay between

\textsuperscript{4}This description of the stationary mean-field density profile describes correctly the situation for \( r = 1 \), but disregards a more complicated sublattice structure for \( r > 1 \). However the figures provided by MacDonald et al.\textsuperscript{[17]} suggest that the description remains qualitatively correct when one averages over this sublattice structure.

\textsuperscript{5}The equivalence to the Heisenberg chain is more obvious after the similarity transformation \( \Phi \) given in the first lecture elsewhere in this volume.
two correlation length which determine the phase diagram and the nature of the phase transitions. In particular, it turns out that the correlation length on the phase transition line between the low-density phase and the high-density phase is infinite, which is incompatible with the mean field result. The exact solution gives a linearly increasing density profile rather than the sharp shock predicted by mean field. This can be explained by assuming that a sharp shock exists, but, due to current fluctuations, performs a random walk along the lattice. Therefore, if one waits long enough, the shock will have been at each lattice with equal probability. This picture yields a linearly increasing density and is confirmed by an exact solution of dynamical properties of a related exclusion process with deterministic bulk dynamics. What one therefore expects for an experimental sample is indeed a region of low density of ribosomes followed by a sharp transition to a region of high density of ribosomes as found experimentally. This rapid increase can be anywhere on the m-RNA, but with a probability distribution given by the effective initialization and release rates $\alpha, \beta$. If $\alpha = \beta$ the distribution of shock position would be constant over the lattice, otherwise exponential on a length scale $\xi = 1/\ln\left[\alpha/(1 - \alpha)/\beta/(1 - \beta)\right]$. If $\alpha, \beta > 1/2$, i.e. when polymerization determines the dynamics, then the exact solution predicts an algebraic decay of the density to its bulk value 1/2 with exponent $b = 1/2$ rather than $b = 1$ predicted by mean field.

4 Exciton Dynamics on Polymer Chains

Finally I would like to discuss briefly an experiment in which excitons on polymer chains are created by laser excitations and then hop on the chain and coagulate when they meet. The carrier substance is $(CH_3)_4NMnCl_3$ (TMMC). The particles are excitons of the $Mn^{2+}$ ion and move along the widely separated $MnCl_3$ chains. A single exciton has a decay time of about $0.7ms$. The on-chain hopping rate is $10^{11} - 10^{12}s^{-1}$. If two excitons arrive on the same $Mn^{2+}$ ion, they undergo a coagulation reaction $A + A \rightarrow A$ with a reaction time $\approx 100fs$.

It has been suggested to describe this process by the coagulation-diffusion model on a one-dimensional lattice which through a similarity transformation is equivalent to the diffusion limited pair annihilation process. In this model each lattice site may be occupied by at most one particle.
These particles hop with rates $D$ to the right or left nearest neighbouring site resp. if this site is vacant and both annihilate with rate $\lambda$ if it is occupied. The annihilation rate is equal to the coagulation rate of the original process. Since the experimental data suggest that the coagulation is approximately instantaneous, one finds $\lambda = D^{25}$. In the quantum Hamiltonian formalism the stochastic time evolution of this transformed process is then given by the Hamiltonian

$$H = -D \sum_{k=1}^{L} \left( s_k^+ s_{k+1}^- + s_k^- s_{k+1}^+ + s_k^+ s_{k+1}^- - \sigma_k^z + 1 \right).$$

(4)

Here $D$ sets the time scale for the diffusion. The finite life time $\tau$ of the excitons is much larger than $D^{-1}$, thus a decay term $\tau^{-1} \sum (s_i^+ - n_i)$ is neglected. This Hamiltonian can be turned by a Jordan-Wigner transformation into an integrable free fermion system. One then finds$^{27}$ that the average density of excitons decays algebraically in time with an exponent $x = 1/2$ in good agreement with the experimental result $x = 0.48(2)^{23}$. The model predicts also an independence of the amplitude of the decay for long times from the initial density as seen in the experiment$^{23, 25}$.

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