Exact stationary state of a staggered stochastic hopping model

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We determine the $N$-particle stationary states of a staggered stochastic hopping model with reflective boundaries. It is shown that the stationary states are in fact so-called optimum ground states. Recursion relations in the particle number for any $l$-point density correlation function will be derived. Furthermore, the connection between reflective boundaries and the occurrence of optimum ground states is examined. An explicit counterexample shows that reflective boundaries do not enforce the stationary state to be an optimum ground state.

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1. INTRODUCTION

Interacting many-particle systems encountered in nature are sometimes difficult to describe in terms of classical or quantum mechanics. A stochastic description is then more appropriate for systems which behave essentially randomly on a phenomenological level. Often this leads to problems far away from thermal equilibrium for which – in contrast to equilibrium systems – a general concept or framework is still missing. Therefore one has to rely on the investigation of special examples. Models which are exactly solvable become then even more important than in equilibrium physics. They allow to probe the nature of non-equilibrium physics with the problems related to the reliability of approximative methods. Also stochastic systems are often used for the modelling of interdisciplinary problems, where the interactions between the entities are not known exactly.

The dynamics of stochastic systems is governed by the master equation

* Dedicated to Prof. Peter Wölfle on the occasion of his sixtieth birthday.
which can be interpreted as a Schrödinger equation in imaginary time (see Sec. 2.). In the analytical treatment of non-equilibrium systems it is therefore possible to exploit this similarity by using successful techniques from equilibrium physics. Especially the so-called matrix product Ansatz (MPA), first developed for spin chains, is important. It has been shown that the stationary state of one-dimensional stochastic processes is generically of MPA-type. However, in most cases it is still very difficult to calculate expectation values explicitly.

In this paper the exact stationary state of a one-dimensional stochastic process with staggered interaction and reflective boundaries is determined. This model can be regarded as the merger of the $U_q[SU(2)]$-symmetric hopping model of Sandow and Schütz and a ratchet model proposed by Kolomeisky and Widom (for details, see ). A similar stochastic hopping model with periodic boundary conditions, where also coagulation and deaggregation processes may occur, has been studied by Fujii using free fermion techniques. Our model can not be solved using free fermion techniques but requires a different approach. This approach relies heavily on the observation that the stationary state of our model is an optimum ground state (OGS). The occurrence of OGS in the context of matrix product states will be elucidated. It will be shown that OGS are not ubiquitous for systems with reflective boundaries.

2. QUANTUM FORMALISM AND DEFINITION OF THE MODEL

We consider stochastic systems on a one-dimensional lattice with $L$ sites. Each cell $j$ can either be empty or occupied by a particle. Its state is characterized by the variable $\alpha_j$ which could e.g. be the occupation number. The model is then defined by its dynamics, namely by the transition rates $w(\alpha \to \beta)$ for a transition from a lattice configuration $\alpha = (\alpha_1, \ldots, \alpha_L)$ to the configuration $\beta = (\beta_1, \ldots, \beta_L)$. The probability $P(\alpha; t)$ to find the system at time $t$ in the configuration $\alpha = (\alpha_1, \ldots, \alpha_L)$ is then given by the master equation

$$\frac{\partial P(\alpha; t)}{\partial t} = \sum_{(\beta)} w(\beta \to \alpha)P(\beta; t) - \sum_{(\beta)} w(\alpha \to \beta)P(\alpha; t).$$

Introducing the state vector $|P(t)\rangle = \sum_{\alpha} P(\alpha_1, \ldots, \alpha_L; t)|\alpha_1, \ldots, \alpha_L\rangle$ the master equation can be written in more compact form

$$\frac{\partial}{\partial t}|P(t)\rangle = -H|P(t)\rangle,$$
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where the matrix elements of the stochastic Hamiltonian $H$ can be expressed through the transition rates $w(\beta \to \alpha)$. For processes with nearest-neighbour interaction and periodic boundary conditions, the stochastic Hamiltonian $H$ can be written as a sum $H = \sum_{j=1}^{L} h_{j,j+1}$ of local Hamiltonians $h_{j,j+1}$ acting only on the sites $j$ and $j + 1$. For other boundary conditions the interactions at the boundaries $j = 1$ and $j = L$ are described by additional boundary operators $h_1$ and $h_L$.

The so-called quantum formalism described above emphasizes the similarity with a Schrödinger equation in imaginary time. The stochastic Hamiltonian $H$, which in general is not hermitean, is often related to spin chains\cite{14}. Therefore it is not surprising that many methods for the treatment of equilibrium systems can be adopted\cite{14}, e.g. free fermion techniques, Bethe Ansatz, or the matrix product Ansatz.

The stationary state $|P\rangle$ reached for $t \to \infty$ is determined by

$$H |P\rangle = 0,$$

i.e. it corresponds to a zero-energy ground state of the Hamiltonian $H$.

In this paper we consider the following stochastic process: Particles with a hard core occupy the sites of a chain of length $L$. The odd sites of the chain belong to sublattice $A$ and the even sites to sublattice $B$. The global stochastic Hamiltonian is an alternating sum of local two-site Hamiltonians

$$H = \sum_{j \in A} \mu_j h_{j,j+1}^A + \sum_{j \in B} \mu_j h_{j,j+1}^B,$$

where $h_{j,j+1}^A$ and $h_{j,j+1}^B$ act non-trivially on sites $j$ and $j + 1$ according to

$$h_{j,j+1}^A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & a & -\frac{1}{a} & 0 \\ 0 & -a & \frac{1}{a} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}_{j,j+1}, \quad h_{j,j+1}^B = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & c & -\frac{1}{c} & 0 \\ 0 & -c & \frac{1}{c} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}_{j,j+1}.$$

The local two-site basis is ordered as follows: \{↑↑, ↑↓, ↓↑, ↓↓\} where ↑ corresponds to an empty site and ↓ to an occupied one. Here we have already used the spin language to emphasize the similarities with spin systems. The only allowed processes are jumps of particles to unoccupied neighbouring sites where the hopping rates alternate along the bonds of the chain.

The $\mu_j \in \mathbb{R}^+$ are arbitrary constants which may differ from site to site. They control the activities of the bonds and influence dynamical properties only.
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3. CONSTRUCTION OF THE STATIONARY STATE

Since no particles enter or leave the chain, the total particle number $N$ is a conserved quantity and the stationary states of a chain of length $L$ can be classified according to the particle number $N \leq L$.

Exact solutions of small systems with $L \leq 4$ indicate that the stationary state for any given particle number is unique and, more interestingly, that this stationary state is an OGS. An OGS is a special type of ground state of a Hamiltonian $H = \sum_{j,l} h_{jl}$, which is at the same time ground state of all local Hamiltonians $h_{jl}$. In the present case this means that all local Hamiltonians $h^{A}_{j,j+1}$ and $h^{B}_{j,j+1}$ have to annihilate the stationary state $\langle P \rangle$ since the “ground state energy” of $H$ is 0 according to (3). Explicitly this has the consequence that if $\langle P \rangle$ has a component $|\alpha_1, \ldots, \alpha_{j-1}, \downarrow, \beta_{j+2}, \ldots, \beta_L \rangle$ it must also have the component $|\alpha_1, \ldots, \alpha_{j-1}, \uparrow, \beta_{j+2}, \ldots, \beta_L \rangle$ with a relative weight given by

$$\{a^{-2}, c^{-2}\}_{j} := \begin{cases} a^{-2} & \text{if } j \text{ odd}, \\ c^{-2} & \text{if } j \text{ even}. \end{cases}$$

Stochastic processes on a one-dimensional lattice with a finite interaction range and boundary interactions have a stationary state which can be written as a matrix product state. This can be shown without using the explicit form of the boundary operators $h_1$, $h_L$. Therefore, reflective boundaries - corresponding to vanishing boundary operators $h_1 = h_L = 0$ - are allowed as well.

A suitable (grand canonical) matrix product ansatz for the stationary state in the presence of staggering has the form

$$|P_L\rangle = \langle W| D \otimes \bar{D} \otimes \cdots \otimes \left\{ D \bar{D} \right\}_L \langle V|,$$

where we have used (6) to write the state for even and odd $L$ in a unified way and

$$D = \begin{pmatrix} E_D \\ \bar{D} \end{pmatrix}, \quad \bar{D} = \begin{pmatrix} \bar{E} \\ D \end{pmatrix}.$$

1In the language of quantum spin chains such boundaries are usually denoted open boundaries.
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$E, D, \bar{E}$ and $\bar{D}$ are matrices acting on some auxiliary vector space $A$, $|V\rangle \in A$ and $\langle W| \in A^*$. By direct computation one verifies that this vector is a ground state of $H$, if one can find matrices $X_1, X_2$ and $\bar{X}_1, \bar{X}_2$, which are the components of the vectors $X$ and $\bar{X}$, respectively, such that the following relations are fulfilled

$$h^A(D \otimes \bar{D}) = X \otimes \bar{D} - D \otimes X,$$
$$h^B(\bar{D} \otimes D) = \bar{X} \otimes D - \bar{D} \otimes X,$$
$$\langle W|X = 0,$$
$$\{X, \bar{X}\}_L |V\rangle = 0.$$  \hspace{1cm} (9)

The most simple way to satisfy this algebra is given by the choice $X_1 = X_2 = \bar{X}_1 = \bar{X}_2 = 0$. Then, the only remaining equations are

$$h^A(D \otimes \bar{D}) = 0,$$
$$h^B(\bar{D} \otimes D) = 0.$$  \hspace{1cm} (10)

turning $|P_L\rangle_0$ into an optimum ground state!

More explicitly, the problem of finding the ground state of $H$ becomes the problem of finding a representation of the quadratic algebra

$$E\bar{D} = \frac{1}{a^2} D\bar{E},$$
$$\bar{E}D = \frac{1}{c^2} \bar{D}E.$$  \hspace{1cm} (11)

The algebra (11) fixes the relative weight of two configurations in $|P_L\rangle_0$ that differ only by the interchange of a particle and a hole at the sites $j$ and $j + 1$. This relative weight is exactly the one that has been proposed above by means of the optimum ground state property given by (6). Thus, in case of reflective boundaries the appearance of optimum ground states can be connected with the fact that the algebra necessary for the construction of the ground state in form of a matrix product state takes its most simple form. Nevertheless, it should be noticed that reflective boundaries do not enforce optimum ground states, as will be shown in the caveat at the end (Sec. 5).

Up to this point, two ways for the construction of the stationary state of $H$ have been presented. The first way gives a recipe for the construction of the relative probabilities of all states that are present in the stationary state. The second way is connected with the matrix product approach: The ground state problem is transformed into the purely algebraic problem of finding the representation of the quadratic algebra (11).
In the following, no use of these two possibilities will be made. Instead, a third way will be given that closely resembles the construction in [12]. The starting point will be the vacuum vector $|\text{vac}\rangle := \prod_{i=1}^{L} |\uparrow\rangle$ describing a completely empty chain.

Out of this vacuum all $N$-particle stationary states will be constructed, using powers of suitable creation operators. With

$$q := \begin{pmatrix} 1 & 0 \\ 0 & ac \end{pmatrix}$$

for every $j \in \{1, 2, \ldots, L\}$ a “local” particle creation operator $b_j^-$ is given by

$$b_j^- = \left[ \left( \frac{1}{a^2} \right)^{\lfloor \frac{j}{2} \rfloor} \left( \frac{1}{c^2} \right)^{\lfloor \frac{j-1}{2} \rfloor} \prod_{i=1}^{j-1} q_i \right] \cdot s_j^-.$$  \hfill (13)

The global creation operator $B^-$ is the sum of all local creation operators

$$B^- = \sum_{j=1}^{L} b_j^-.$$  \hfill (14)

In order to shorten the notation one furthermore defines

$$\{k\}_{a,c} := \left( \frac{1}{a^2} \right)^{\lfloor \frac{k}{2} \rfloor} \left( \frac{1}{c^2} \right)^{\lfloor \frac{k-1}{2} \rfloor}, \quad [k]_{a,c} := \frac{1 - (ac)^k}{1 - ac},$$

$$[k]_{a,c}! := [1]_{a,c}[2]_{a,c} \cdots [k]_{a,c}.$$  \hfill (15)

The symbol $\{k\}_{a,c}$ should not be confused with $\left\{ \frac{a-2}{c-2} \right\}_j$ defined in [3], which looks similar but has a different meaning. The floor function $\lfloor k \rfloor$ denotes the largest integer $\leq k$. With these definitions the unnormalized $N$-particle stationary state $|N\rangle$ is built out of the vacuum by

$$|N\rangle := \frac{1}{[N]_{a,c}!} (B^-)^N |\text{vac}\rangle.$$  \hfill (16)

In addition, one has the left complete $N$-particle state, defined as

$$\langle N | := \langle \text{vac} | \frac{1}{N!} (S^+)^N.$$  \hfill (17)

Note that creation of particles corresponds to lowering a spin in the language of spin-operators.
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For the left complete state it is straightforward to show that

\[ \langle N| s_k^- = \langle N-1|(1-n_k). \]  

(18)

From exact solutions of systems with \( L \leq 4 \) a similar relation has been guessed for the unnormalized \( N \)-particle state \( |N\rangle \): For all \( k \in \{1, 2, \ldots , L\} \) the following identity holds

\[ s_k^+|N\rangle = \{k\}_{a,c}(1-n_k)|N-1\rangle \]  

(19)

which can be proven by direct calculation. As a consequence one finds that the \( l \)-point density correlation functions obey the recursion relation

\[ \langle N|n_{x_1} \ldots n_{x_l}|N\rangle = \{x_l\}_{a,c}\langle N-1|n_{x_1} \ldots (1-n_{x_l})|N-1\rangle. \]  

(20)

With this recursion relation at hand it is easy to prove that

\[ P(\alpha_1, \ldots, \alpha_{k-1}, \uparrow, \downarrow, \beta_{k+2}, \ldots, \beta_L) \]  

\[ P(\alpha_1, \ldots, \alpha_{k-1}, \downarrow, \uparrow, \beta_{k+2}, \ldots, \beta_L) = \begin{cases} a^{-2} \\ c^{-2} \end{cases} \]  

(21)

which suffices to show that the \( N \)-particle states defined above are optimum ground states and hence stationary states.

Note that \( B^- \) does not commute with \( H \) and so does not reflect a global symmetry. Both operators commute only, if they are restricted to the kernel of \( H \). Therefore, the integrability found for \( a = c = q \) is most presumably lost if \( a \neq c \).

4. DENSITY PROFILES FROM RECURSION RELATIONS

For the calculation of density profiles, in principle, the normalization of \( |N\rangle \) has to be computed. Unfortunately, a direct computation of this quantity is very involved and tedious. Therefore a step-by-step method has been chosen. Assume that \( Z(N-1) \) is the normalization of \( |N-1\rangle \). Assume further that \( z_N \) is such that the normalization \( Z(N) \) of \( |N\rangle \) is given by

\[ Z(N) = z_N Z(N-1). \]  

(22)

This gives with (20)

\[ \rho_k(N) = \frac{\langle N|n_k|N\rangle}{Z(N)} = \frac{\{k\}_{a,c}}{z_N}(1 - \rho_k(N-1)). \]  

(23)

In the \( N \)-particle state naturally the identity \( \sum_{k=1}^{L} \rho_k(N) = N \) holds. Thus,

\[ z_N = \frac{1}{N} \sum_{k=1}^{L} \{k\}_{a,c}(1 - \rho_k(N-1)). \]  

(24)
Finally, one finds a recursion relation for the local density of an $N$-particle stationary state

$$\rho_k(N) = N \frac{\{k\}_{a,c}(1 - \rho_k(N - 1))}{\sum_{j=1}^{L} \{j\}_{a,c}(1 - \rho_j(N - 1))}. \quad (25)$$

Starting from the normalized stationary state $|\text{vac}\rangle$, which belongs to $N = 0$ and has $\rho_k(0) = 0$, the density profiles for all $N$ can be computed. The results have been compared with Monte Carlo data (see Fig. 1 and Fig. 2) showing perfect agreement. Generically we find exponentially decaying density profiles. If one of the parameters is larger than one, whereas the other parameter is smaller than one, the density profiles clearly reflect the sublattice structure of the Hamiltonian, since the slope of the profile is alternatingly positive and negative along the bonds (see Fig. 1). The shape of the density profile can be explained qualitatively in the following way: on the odd bonds hopping to the right is favoured because $a^{-1} = 2$ and $a = 1/2$. As a consequence, the density at the left end of an odd bond is smaller than the density at the right end. Along the even bonds one has the opposite scenario since $c = 5/2$ and $c^{-1} = 2/5$. Finally, the high density in the left part of the
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![Graph showing density profile](image)

Fig. 2. Density profile of staggered hopping-model. \( a = 2.0, \ c = 4.0, \ L = 50 \) and \( N = 10 \). The dashed line corresponds to analytical data from \(^{(25)}\). The boxes represent Monte Carlo data.

system is due to the fact that the maximal hopping amplitude can be found at the even bonds which favour hopping to the left.

If both parameters \( a \) and \( c \) are larger or smaller than one, we find a different behaviour. Now the density profiles become monotonous functions of \( \rho \) and the sublattice structure is hidden (see Fig. 2).

5. A CAVEAT

As presented above, optimum ground states come into play naturally if one encounters stochastic processes with reflective boundaries. Therefore one might conjecture that the stationary state of such processes is always of this special type. However, this is not true. In the following a \( \mathbb{Z}_3 \)-symmetric reaction-diffusion model will be presented, which has zero-energy ground states that are not (always) optimum ground states.

The sites of a chain of length \( L \) are coloured with the elements of \( \mathbb{Z}_3 \), i.e., one has three types of particles \( (k = 0, 1, 2) \) on a completely filled chain. Two particles on neighbouring sites react according to the following rules
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(algebraic manipulations are done according to $\mathbb{Z}_3$)

\[
\begin{align*}
(k, k + 1) &\rightarrow (k + 1, k) \quad \text{with rate } \alpha, \\
(k, k + 2) &\rightarrow (k + 1, k + 1) \quad \text{with rate } \beta.
\end{align*}
\]

Thus, the local Hamiltonian is given by

\[
h = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\beta & 0 \\
0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \beta & 0 & 0 & 0 & 0 & 0 & \alpha \\
0 & -\alpha & 0 & \beta & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\beta & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\alpha & 0 & \beta & 0 & 0 \\
0 & 0 & 0 & -\beta & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.
\]

The operators $h_{j,j+1}$ act as $h$ on sites $j, j+1$ and as identity on the remaining sites of the chain, and hence the global stochastic Hamiltonian reads

\[
H = \sum_{j=1}^{L-1} h_{j,j+1}.
\]

The exact solution for $L = 2$ shows a threefold degenerate ground state

\[
|\psi\rangle_2 = |k, k\rangle \text{ with } k \in \mathbb{Z}_3.
\]

These states are optimum ground states.

Looking at $L = 3$ a new situation arises. One has again a threefold optimum ground state

\[
|\psi\rangle_3 = |k, k, k\rangle \text{ with } k \in \mathbb{Z}_3.
\]

In addition, one finds two qualitatively different ground states

\[
|\varphi_1\rangle_3 = \sum_{k \in \mathbb{Z}_3} \left[ |k, k, k + 2\rangle + \frac{\beta}{\alpha} |k, k + 1, k + 1\rangle + \frac{\beta}{\alpha + \beta} |k, k + 2, k\rangle \right],
\]

\[
|\varphi_2\rangle_3 = \sum_{k \in \mathbb{Z}_3} \left[ |k, k + 2, k + 2\rangle + \frac{\beta}{\alpha} |k, k, k + 1\rangle + \frac{\beta}{\alpha + \beta} |k, k + 1, k\rangle \right].
\]

These states are not optimum ground states. Moreover

\[
h_{1,2}|\varphi_j\rangle_3 = -h_{2,3}|\varphi_j\rangle_3 \neq 0 \quad \text{with } j = 1, 2.
\]
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The occurrence of such states might be connected with the existence of an additional symmetry.

The last result can also be understood in the context of MPA. As the two additional states are not optimum ground states, the cancelling vector $\mathcal{X}$ has to be nontrivial. Therefore,

$$|\varphi_j\rangle_3 = \langle W|D \otimes D \otimes D|V\rangle.$$ (33)

Using the fact that $\langle W|$ and $|V\rangle$ must be in the kernel of $\mathcal{X}$ one finds

$$h_{1,2}\langle W|D \otimes D \otimes D|V\rangle = -\langle W|D \otimes \mathcal{X} \otimes D|V\rangle,$$
$$h_{2,3}\langle W|D \otimes D \otimes D|V\rangle = \langle W|D \otimes \mathcal{X} \otimes D|V\rangle,$$ (34)

and thus (32) holds.

Most interestingly systems of length $L = 4$ and $L = 5$ – like the two-site system – possess only threefold degenerate optimum ground states. But then, for $L = 6$, two additional ground states show up again. This might be related to an additional symmetry occurring for system sizes which are an integer multiple of three.

This example shows that reflective boundary conditions do not imply the existence of an OGS. However, it still leaves open the possibility that systems with reflecting boundary conditions and a unique stationary state have optimum ground states.

6. CONCLUSIONS

We have presented the exact solution for the stationary state of a stochastic process with staggered hopping rates. Using the similarity of the quantum formalism to the master equation the model could be interpreted as a spin chain. Its ground state – corresponding to the stationary state of the stochastic process – was shown to be an optimum ground state, i.e. it is at the same time ground state of all local Hamiltonians $h_{j,j+1}$ which make up $H$. Furthermore the $l$-point density correlation functions have been determined recursively.

Apart from the fact that the model is one of the very few exactly solvable models with staggered interactions it might have practical applications. A similar model has been proposed by Kolomeisky and Widom17. It is a simplified ratchet model (for a recent review, see23) for molecular motors effectively describing the motion of a motor protein on a micro-tubule24.
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