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On the existence of a phase transition for an exclusion process on a ring

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Abstract
We study the stationary state of a simple exclusion process on a ring which was introduced by Arndt *et al*. In a previous study by Rajewsky *et al* it was claimed that the spatial particle condensation the model exhibits is not associated with a phase transition in the framework of a grand canonical ensemble. The discussions were, however, based on an assumption about the monotonicity of a certain function appearing in the analysis. In this paper we prove the assertion. The proof combined with the previous discussions shows convincingly that there is no phase transition in the framework of a grand canonical ensemble.

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1. Introduction

Over the last decade, one-dimensional driven diffusive systems have proved to be quite useful models in the study of non-equilibrium statistical physics. Typically, in such a system, one considers the dynamics of several species of particles on a one-dimensional chain, where particles hop and interchange their positions with prescribed rates. The most well-studied process among these is the asymmetric simple exclusion process (ASEP), where there is only one species of particle (two possible states per site). Whereas the ASEP is a very simple model which admits exact mathematical analysis, it already exhibits rich non-equilibrium behaviours such as boundary-induced phase transition, anisotropic critical phenomena and so on. More recently, it has been noted that the models with more than one species of particle show equally interesting and sometimes more intriguing phenomena.

In the papers [1, 2] (see also a recent preprint [3]), a particular model with two species of particles (three possible states per site) was introduced and studied which appeared numerically to show a phase transition. The stationary properties of the process crucially depends on the particle density. Above a certain initial density, the system shows a particle condensation,

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while below this threshold density the stationary state is disordered. As a consequence, the current as a function of the particle density seems to be non-differentiable. Hence one expects the existence of a phase transition.

However, in [4], it was suggested that this was not in fact a correct analytical description of the situation: the stationary properties of the system depends analytically on the density, meaning that there is no phase transition in the strict sense of the word. The condensation mentioned above never happens, but instead there is a very rapid change of scale of the system as the density varies over an extremely narrow range, so that the breakdown of the particle condensation cannot be seen unless one looks at huge systems (in a typical example with a lattice size of the order 10^{70} for quite reasonable values of the parameters).

The argument in [4], and hence the correctness of its consequences, is essentially based on an assumption about the monotonicity of a certain function $f(y)$. This function determines the thermodynamic behaviours of the model and its monotonicity is essential for the analyticity of physical quantities in the thermodynamic limit. The purpose of this paper is to give a proof of the monotonicity assertion. We point out that there are still a few other questions concerning the argument in [4]. The most outstanding issue is the equivalence of ensembles. The above-mentioned particle condensation is observed in a canonical ensemble; the number of particles is conserved in computer simulations. On the other hand, most of the analysis in [4] was carried out in a grand canonical ensemble which is a superposition of canonical ensembles with various numbers of particles. Hence, in order for the argument in [4] to be valid for the description of the particle condensation observed in computer simulations, the equivalence of ensembles should be established. A heuristic argument supporting its validity is already given in [4], but there is no proof for the moment. Anyway, the discussions in [4] combined with the proof in this paper provide strong evidence that the particle condensation observed in this process is not associated with a phase transition, at least in the framework of a grand canonical ensemble.

We now formulate the precise mathematical statement. First we introduce some notations:

$$(z;q)_n = \begin{cases} 1 & \text{if} \quad n=0 \\ (1-z)(1-zq)(1-zq^2)\cdots(1-zq^{n-1}) & \text{if} \quad n>0 \end{cases}$$

$$(z;q)_\infty = \prod_{n=0}^{\infty}(1-zq^n)$$

$$(a_1,a_2,\ldots,a_k;q)_n = (a_1;q)_n(a_2;q)_n\cdots(a_k;q)_n$$

$$(a_1,a_2,\ldots,a_k;q)_\infty = (a_1;q)_\infty(a_2;q)_\infty\cdots(a_k;q)_\infty.$$

The above-mentioned function $f(y) = f(a,b;q;y)$ is defined by

$$f(y) = y\frac{(qy^2,q;q)_\infty}{(ay,by;q)_\infty}\sum_{n=0}^{\infty}\frac{(ay,by;q)_n}{(qy^2,q;q)_n}q^n. \tag{1.1}$$

In [4], we considered the special case where $a=b$ holds. The proof of the original assertion in [4] will be obtained by merely setting $a=b$ in the following statements. In this paper, we restrict our attention to the case $a,b,q\in(-1,1)$. Though the physical meaning of the model with negative values of q is unclear, it is irrelevant in the following mathematical discussion. The results we prove are the following.

Theorem 1. *The derivative of $f(y)$ is positive;*

$$f'(y) > 0$$

for all $a,b,q\in(-1,1)$ and $0\leqslant y\leqslant 1$.

Remark. Since it is easy to see that

$$f'(0) = (q;q)_\infty \sum_{n=0}^{\infty} \frac{q^n}{(q;q)_n} = 1$$

we take $0 < y \leqslant 1$ in what follows.

Theorem 2. *The derivative of $f(y)$ at $y = 1$ is given by*

$$f'(1) = \frac{(ab;q)_\infty (q;q)_\infty^3}{(a,b;q)_\infty^2}. \tag{1.2}$$

Remark. The special case $a = b = -q$ of (1.2) was already proved in [4].

To prove these theorems, we need some knowledge from the theory of orthogonal polynomials. In section 2, after explaining these, we give an integral representation of f which allows us to prove both theorems quite easily. On the other hand, for theorem 2, we can also give a more direct and self-contained proof. This is done in section 3. Finally, in section 4 we mention some asymptotic formulae for $f'(1)$ which follow from (1.2) and explain the surprising numerical results of [1, 2].

2. The Al-Salam–Chihara polynomials

2.1. Some facts from the theory of orthogonal polynomials

In this section, we quote some relevant known facts without proofs. In the theory of orthogonal polynomials, real, symmetric, tridiagonal matrices with positive off-diagonal entries are called Jacobi matrices. Hence a Jacobi matrix T has the form

$$T = \begin{bmatrix} a_1 & b_1 & 0 & 0 & \cdots \\ b_1 & a_2 & b_2 & 0 & \\ 0 & b_2 & a_3 & b_3 & \\ \vdots & & \ddots & \ddots & \ddots \end{bmatrix} \qquad b_n > 0 \quad (n = 1, 2, \ldots). \tag{2.1}$$

Using the matrix elements of T, we define a set of polynomials by $p_0(t) = 1$, $p_1(t) = (t - a_1)/b_1$ and

$$t p_n(t) = b_n p_{n-1}(t) + a_{n+1} p_n(t) + b_{n+1} p_{n+1}(t) \qquad (n \geqslant 1).$$

Let us denote $\langle 0| = (1\,0\,0\,\ldots)$ and $|0\rangle = \langle 0|^T$, where the superscript T indicates the transpose. Then the following is a fundamental theorem in the general theory of orthogonal polynomials (see, for instance, [5]).

Theorem 3. *Associated with a bounded Jacobi matrix T, there exists a unique probability measure $\mathrm{d}\mu$ on $\mathbb{R}$ with compact support such that*

$$\langle 0| \frac{1}{x - T} |0\rangle = \int \frac{\mathrm{d}\mu\,(t)}{x - t} \qquad \mathrm{Im}\,(x) \neq 0.$$

Moreover, the set of polynomials $\{p_n\}_{n \geqslant 0}$ is orthonormal with respect to this measure $\mathrm{d}\mu$, i.e.

$$\int p_m(t) p_n(t)\,\mathrm{d}\mu\,(t) = \delta_{m,n}.$$

Next we consider a Jacobi matrix of a more specific form for which the a_n and b_n in (2.1) are given by

$$a_n = (a+b)q^{n-1}$$
$$b_n = \sqrt{(1-q^n)(1-abq^{n-1})}.$$

We remark here that the boundedness of the Jacobi matrix is easily shown for this choice of the matrix elements when $a, b, q \in (-1, 1)$. As pointed out in [4, 6], the orthogonal polynomials associated with this Jacobi matrix are known as Al-Salam–Chihara polynomials in the literature [7, 8]. The corresponding measure with respect to which these polynomials are orthogonal was obtained in [7]. For the range of parameters of present interest, the measure is absolutely continuous and has the form $\mathrm{d}\mu(t) = \frac{\sqrt{4-t^2}}{2\pi} F(t)\,\mathrm{d}t$ where the weight function $F(t)$ is defined by

$$F(t) = \begin{cases} (q, ab; q)_\infty \prod_{n=0}^{\infty} \dfrac{1-(t^2-2)q^{n+1}+q^{2n+2}}{(1-atq^n+a^2q^{2n})(1-btq^n+b^2q^{2n})} & (|t| \leqslant 2) \\ 0 & \text{otherwise.} \end{cases} \tag{2.2}$$

2.2. *Proof of theorems*

In [4], we defined a function $\chi(x)$ by

$$\chi(x) = \langle 0| \frac{1}{x-2-T} |0\rangle$$

and gave an expression of χ in terms of f:

$$\chi(x) = f(y(x)) \tag{2.3}$$

with

$$y(x) = \frac{x-2-\sqrt{x^2-4x}}{2}.$$

On the other hand, from theorem 3, the function $\chi(x)$ also has the integral representation,

$$\chi(x) = \frac{1}{2\pi} \int_{-2}^{2} \frac{\sqrt{4-t^2}F(t)}{x-2-t}\,\mathrm{d}t \tag{2.4}$$

with the function $F(t)$ given by (2.2). It is now quite simple to prove theorems 1 and 2.

Proof of theorem 1. Combining the two different representations, (2.3) and (2.4), of the function $\chi(x)$, we see that f has the integral representation,

$$f(\mathrm{e}^{-u}) = \frac{1}{\pi} \int_0^\pi F(2\cos\theta)\,\frac{\sin^2\theta\,\mathrm{d}\theta}{\cosh u - \cos\theta}. \tag{2.5}$$

Since $F(t)$ is positive, it is clear that the right-hand side of (2.5) is a monotone decreasing function of $u \in (0, \infty)$.

Proof of theorem 2. Differentiating (2.5) and setting $\theta = tu$, we find

$$\begin{aligned} \mathrm{e}^{-u} f'(\mathrm{e}^{-u}) &= \frac{\sinh u}{\pi} \int_0^\pi F(2\cos\theta)\,\frac{\sin^2\theta\,\mathrm{d}\theta}{(\cosh u - \cos\theta)^2} \\ &= \frac{1}{4\pi} \int_0^{\pi/u} F(2\cos(tu))\,\frac{u\,\sinh(u)\,\sin^2(tu)\,\mathrm{d}t}{(\sin^2(tu/2)+\sinh^2(u/2))^2} \end{aligned}$$

and hence, letting u tend to zero and using formula (2.2),

$$f'(1) = \frac{4}{\pi} F(2) \int_0^\infty \frac{t^2\,\mathrm{d}t}{(t^2+1)^2} = F(2) = \frac{(q, q, q, ab; q)_\infty}{(a, a, b, b; q)_\infty}.$$

3. Alternative proof of theorem 2

The proofs given in the last section are complete, but make use of fairly advanced results from the literature. In this section, we give a more direct and elementary proof of theorem 2. The method would also be applicable to the analysis of a wider class of models.

If we introduce the basic hypergeometric function [9]

$$ {}_2\phi_1\left[\begin{array}{c} a_1, a_2 \\ b \end{array}; q, z\right] = \sum_{n=0}^{\infty} \frac{(a_1, a_2; q)_n}{(b, q; q)_n} z^n $$

then (1.1) is rewritten as

$$ f(y) = y\frac{(qy^2, q; q)_\infty}{(ay, by; q)_\infty} {}_2\phi_1\left[\begin{array}{c} ay, by \\ qy^2 \end{array}; q, q\right]. $$

Using the formula for ${}_2\phi_1$ [9],

$$ {}_2\phi_1\left[\begin{array}{c} a_1, a_2 \\ b \end{array}; q, z\right] = \frac{(a_2, a_1 z; q)_\infty}{(b, z; q)_\infty} {}_2\phi_1\left[\begin{array}{c} b/a_2, z \\ a_1 z \end{array}; q, a_2\right] $$

we find that the function f has an alternative formula,

$$ f(y) = \sum_{n=0}^{\infty} \frac{(b^{-1}qy; q)_n}{(ay; q)_{n+1}} b^n y^{n+1}. $$

From this we deduce that $f'(1) = g(a, b)$, where

$$ g(a, b) = g(a, b; q) = \sum_{n=0}^{\infty} \frac{(b^{-1}q; q)_n}{(a; q)_{n+1}} b^n \left\{ \sum_{r=-n}^{-1} \frac{1}{1 - bq^r} + \sum_{r=0}^{n} \frac{1}{1 - aq^r} \right\}. \tag{3.1} $$

We have to prove that $g(a, b)$ is equal to the right-hand side of (1.2). We do this by showing that g satisfies the recursion

$$ g(aq, b) = \frac{(1-a)^2}{1-ab} g(a, b). \tag{3.2} $$

From the symmetry between a and b of $f(y)$ (which is manifest in the expression (1.1)) and hence of $g(a, b)$, we also have

$$ g(a, bq) = \frac{(1-b)^2}{1-ab} g(a, b). $$

These two recursions imply that $g(a, b) = C(q)(ab; q)_\infty/(a, b; q)_\infty^2$ for some constant $C(q)$. Setting $a = b = 0$ gives $C(q) = g(0, 0) = \sum_{n=0}^{\infty}(-1)^n(2n+1)q^{\frac{n(n+1)}{2}} = (q; q)_\infty^3$ and hence (1.2).

To prove the recursion (3.2), we rewrite equation (3.1) as

$$ g(a, b) = \sum_{n=0}^{\infty} U_n(a, b)\left\{\phi(bq^{-1}) - \phi(bq^{-n-1}) + \phi(aq^n) - \phi(aq^{-1})\right\} $$

where we have set $U_n(a, b) = \frac{(b^{-1}q;q)_n b^n}{(a;q)_{n+1}}$ and $\phi(x) = \sum_{r=0}^{\infty} \frac{1}{1-q^{-r}x}$. From the easily established recursions $\frac{1-ab}{1-a} U_n(aq, b) = U_n(a, b) - aU_{n+1}(a, b)$ and $\phi(qx) = \frac{1}{1-qx} + \phi(x)$ we find

$$ \begin{aligned} \frac{1-ab}{1-a} g(aq, b) &= \sum_{n=0}^{\infty}(U_n(a, b) - aU_{n+1}(a, b))\left\{\phi(bq^{-1}) - \phi(bq^{-n-1}) + \phi(aq^{n+1}) - \phi(a)\right\} \\ &= (1-a)g(a, b) + \sum_{n=0}^{\infty} U_n(a, b)\left(\frac{1}{1-aq^{n+1}} + \frac{a}{1-bq^{-n}}\right) - \frac{a}{(1-a)(1-b)} \\ &\quad - \sum_{n=0}^{\infty} U_n(a, b). \end{aligned} $$

However, on the right-hand side, all the terms other than $(1-a)g(a,b)$ cancel since $U_0(a,b) = \frac{1}{1-a}$ and $U_n(a,b) = \frac{U_n(a,b)}{1-aq^{n+1}} + \frac{aU_{n+1}(a,b)}{1-bq^{-n-1}}$ for $n \geqslant 0$. This establishes (3.2).

4. Asymptotics of $f'(1)$

From the formula for $f'(1) = g(a,b;q)$ given in theorem 2 we can deduce the asymptotic behaviour of this function for q tending to 1, thus obtaining a quantitative explanation of the phenomena discovered in [1,2]. For simplicity we state the results only in the case $a = b$.

Proposition 1. *The asymptotics of $g(a;q) = g(a,a;q)$ for $q = \mathrm{e}^{-t}$ with t tending to zero and $a = 0$ or $a = \pm\mathrm{e}^{-\lambda t}$ ($\lambda > 0$ fixed) are given by*

$$g(-\mathrm{e}^{-\lambda t};\mathrm{e}^{-t}) = \frac{2^{4\lambda}\pi^2}{\Gamma(2\lambda)}\,t^{-2\lambda-1}\,\mathrm{e}^{-\pi^2/t}\left(1+\frac{\lambda}{2}\,t+\cdots\right)$$
$$g(0;\mathrm{e}^{-t}) = (2\pi)^{3/2}\,t^{-3/2}\,\mathrm{e}^{-\pi^2/2t}\left(1+\tfrac{1}{8}\,t+\cdots\right)$$
$$g(\mathrm{e}^{-\lambda t};\mathrm{e}^{-t}) = \frac{\Gamma(\lambda)^4}{\Gamma(2\lambda)}\,t^{2\lambda-3}\left(1+\frac{\lambda}{2}\,t+\cdots\right).$$

Proof. These results, and indeed the complete asymptotic expansions in powers of t, follow from formula (1.2) for $g(a;q)$ and from the asymptotic expansion

$$\prod_{n=0}^{\infty}\left(1-q^n x\right) \sim \frac{(2\pi)^{1/2}}{\Gamma(\lambda)}\,t^{-\lambda+\frac{1}{2}}\,\exp\left(-\frac{\pi^2}{6t}-\sum_{r=1}^{\infty}\frac{B_r}{r}\,\frac{B_{r+1}(\lambda)}{(r+1)!}\,t^r\right) \qquad (4.3)$$

valid for $x = q^\lambda$ with λ fixed and $q = \mathrm{e}^{-t}$ tending to 1, where $B_n(y)$ denotes the nth Bernoulli polynomial (defined by $\int_x^{x+1} B_n(y)\,\mathrm{d}y = x^n$) and $B_n = B_n(0)$ the nth Bernoulli number. To get the result for $a = -\mathrm{e}^{-\lambda t}$ in proposition 1, we also need the asymptotic formula for $\prod_{n=0}^{\infty}(1+q^{\lambda+n})$, which can be obtained from (4.3) by writing $1+q^{\lambda+n} = (1-q^{2(\lambda+n)})/(1-q^{\lambda+n})$. □

The formula (4.3) is in principle well known, but for the reader's convenience we sketch its proof. The easily obtained 'shifted' version of the classical Euler–Maclaurin summation formula implies the asymptotic expansion

$$\sum_{n=0}^{N-1} f((n+\lambda)t) \sim \frac{1}{t}\int_0^{Nt} f(x)\,\mathrm{d}x + \sum_{r=0}^{\infty}\frac{B_{r+1}(\lambda)}{(r+1)!}\,(f^{(r)}(Nt)-f^{(r)}(0))\,t^r \qquad (t\to 0) \qquad (4.4)$$

valid for λ fixed and for any function $f(x)$ which is smooth on $[0,\infty)$. For our purpose, we need another variant of the Euler–Maclaurin summation formula,

$$\sum_{n=0}^{\infty} f((n+\lambda)t) \sim \frac{1}{t}\int_0^{\infty} f(x)\,\mathrm{d}x + C\left[\left(\frac{1}{2}-\lambda\right)\log t+\frac{1}{2}\log(2\pi)-\log\Gamma(\lambda)\right]$$
$$-\sum_{r=0}^{\infty}\frac{B_{r+1}(\lambda)}{r+1}\,c_r\,t^r \qquad (t\to 0) \qquad (4.5)$$

valid for a fixed value of λ and for $f(x)$ which rapidly decays at infinity and has an asymptotic expansion $f(x) \sim C\log x + \sum_{r=0}^{\infty} c_r x^r$ as $x \to 0$. This is obtained by applying (4.4) to $f(x) - C\log x$ and then taking the limit $N \to \infty$. We apply (4.5) to $f(x) = \log(1-\mathrm{e}^{-x})$ and obtain (4.3) after a short computation.

From proposition 1 it follows that $g(a; q)$ is extremely small for q near to 1 and $a \leqslant 0$, typical numerical examples being

$$g(-\tfrac{4}{5}; \tfrac{5}{6}) \approx 2.8 \times 10^{-19}$$
$$g(-0.95; 0.95) \approx 3.3 \times 10^{-78}$$
$$g(-0.99; 0.99) \approx 5.1 \times 10^{-419}.$$

It is this phenomenon which led to the misleading apparent implications about phase transitions of the numerical simulations presented in [1, 2].

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