Spatial Particle Condensation 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 recently introduced by Arndt et al [14, 15]. This model exhibits spatial condensation of particles. It has been argued [14, 15] that the model has a phase transition from a “mixed phase” to a “disordered phase”. However, in this paper exact calculations are presented which, we believe, show that in the framework of a grand canonical ensemble there is no such phase transition. An analysis of the fluctuations in the particle density strongly suggests that the same result also holds for the canonical ensemble.

1 Introduction

One-dimensional driven diffusive systems have attracted the interest of researchers in a wide variety of fields, including mathematics, physics, chemistry and biology [1–4]. One of

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the most basic of these models is the asymmetric simple exclusion process (ASEP), which already exhibits a rich behavior. Within physics, for example, the ASEP has been used to study boundary induced phase transition \cite{5}, spontaneous symmetry breaking \cite{6}, phase separation \cite{7} and shocks \cite{8,9}. As one of the few models in non-equilibrium physics which is analytically accessible, it has served as a laboratory to test basic concepts of statistical mechanics for far from equilibrium systems. Moreover, its simplicity has led to applications in such diverse fields as the kinetics of biopolymerization \cite{10}, vehicular traffic \cite{11,12} and, most recently, sequence alignment problems in biology \cite{13}.

In this paper, we study a related exclusion process which exhibits a spatial condensation of particles. This model was introduced by Arndt, Heinzl and Rittenberg \cite{14,15} and will be called AHR model below.

In the AHR model two types of particles, called positive and negative, occupy the sites of a periodic one-dimensional lattice of length $L$. The particles are subject to hard-core exclusion, so that there are three possible states at each site: empty, occupied by a positive particle, or occupied by a negative particle. Positive particles hop at rate $\alpha$ into empty spaces (holes) to their immediate right, and negative particles at the same rate into empty spaces to their left. Adjacent positive and negative particles also exchange positions with asymmetric rates $p_R$ and $p_L$. Specifically, the rules are

$$
+ 0 \rightarrow 0 + \text{ with rate } \alpha, \\
0 - \rightarrow - 0 \text{ with rate } \alpha, \\
+ - \rightarrow - + \text{ with rate } p_R, \\
- + \rightarrow + - \text{ with rate } p_L;
$$

we assume that $p_R, \alpha > 0$ and $p_L \geq 0$. A key parameter in the model is ratio of $p_L$ to $p_R$, which we denote by $q$: $q = p_L/p_R$. Our notation here is not that of \cite{14,15}, where $q$ denotes the inverse of this ratio; we adopt this change to agree with the standard notation in the theory of basic hypergeometric functions (see e.g. \cite{16}). Finally, we normalize our time scale by setting $p_R = 1$, so that the rates for exchange of positive and negative particles are 1 and $q$. Note that the numbers $N_\pm$ of positive and negative particles are constants of the dynamics; we will write $\rho_\pm = N_\pm/L$ for the particle densities.

We remark that when $p_L = 0$ and $p_R = \alpha = 1$ the model corresponds to a two-species ASEP (with “first” and “second class” particles) which has been solved in \cite{8}. The system with no holes ($N_+ + N_- = L$) corresponds to the partially asymmetric exclusion process on a ring, for which the stationary measure is trivial (all configurations are equally likely).

The stationary state of the AHR model displays a rich dynamical behavior, which was extensively investigated in \cite{14,17}. Two methods were used: Monte Carlo simulations were carried out in the canonical ensemble (CE), in which the numbers $N_\pm$ of particles are fixed, and analytic calculations (still in finite systems) using a quadratic algebra were carried out in a grand canonical ensemble (GCE), in which the densities are controlled by fugacities $\xi_\pm$ and can fluctuate. These results were then extrapolated to infinite volume. Most of the work was done in the case of equal densities ($N_+ = N_-$ or $\zeta_+ = \zeta_-), which is the only case we will consider here.
These investigations strongly suggest the existence of three different phases for the model, differing in the nature of typical spatial particle configurations (see Figure 1 for space-time representations). We summarize the discussion of [14, 15] and the nomenclature adopted there. For $q > 1$ the system is in the “pure phase”: typical configurations contain three blocks, one each of holes, positive particles, and negative particles. In the thermodynamic limit ($L \to \infty$) the current vanishes. The system in this phase is closely related to a class of models studied in [8]. For $0 \leq q < 1$ the phase depends on the density $\rho = \rho_+ = \rho_-$. For relatively small densities, density profiles of both species are uniform and there is no spatial condensation (the “disordered phase”). For larger densities one observes the formation of a condensate made of $+$ and $-$ particles (with some holes at the boundaries); a block of holes, occasionally traversed by $+$ or $-$ particles, occupies the rest of the system (the “mixed phase”). At the transition between the mixed and disordered phases the Monte Carlo simulations suggest that the infinite volume current $J$ of $+$ particles increases monotonically from zero to a value $(1-q)/4$ as the the density $\rho$ increases from zero to a certain value $\rho_c$, and then takes the constant value $(1-q)/4$ for $\rho_c < \rho < 1/2$ (see Figure 8 of [15]). This indicates that the function $J(\rho)$ is non-analytic—in fact, the simulations suggest it is not differentiable—at a certain value of density $\rho_c$. The same apparent non-analyticity is seen in plots, derived from calculations in the GCE, of $J$ as a function of $q$ at fixed $\rho$ (Figures 1 and 2 of [15]). This would correspond to a “phase transition” in the language of equilibrium physics.

In fact, however, we believe that our analysis shows that these numerical results are misleading. Our main result is an explicit exact formula for the current $J$ in the infinite system in the framework of a GCE. This computation was possible because the AHR model is closely related to the one-dimensional partially asymmetric simple exclusion processes, for which recently analytic exact expressions for various expectation values have been computed [17–19]. It turns out that if $q < 1$ then the current $J(\rho)$ is analytic everywhere, although the derivative of $J(\rho)$ changes very rapidly as $\rho$ passes $\rho_c$ when $q$ is close to one. This strongly suggests that in the GCE, there is no phase transition. For this reason, we will here speak of the mixed regime and the disordered regime, and refer to the union of these regimes as the mixed/disordered phase.

Now, is this also true for the CE? Based on the observation that the density fluctuations in the GCE go to zero in the thermodynamic limit, we believe that the answer to this question is yes, although the argument is not rigorous (See section 5 for a more detailed discussion.)

The existence of a phase transition between the pure and the mixed/disordered phase seems uncontroversial [14, 15] and will not be discussed in the following. Therefore, $q$ is normally chosen to satisfy $0 \leq q < 1$ from now on, although we will occasionally consider $q = 1$ as a special limiting case.

This paper is organized as follows. In section 2, we present the basic structure of the exact solution and define the GCE and CE. The current and density in the GCE are computed in section 3. An analysis of the model when $q$ is close to one is carried out in section 4. In section 5 we discuss to what extent the results for the GCE are valid for the CE. The final section contains our conclusions.
2 Exact solution of the stationary state

The stationary state of the AHR model can be constructed by applying the so-called matrix product ansatz (MPA) \[20, 21\]; this is the method used for the grand canonical calculations in \[14, 15\]. Since its original application to the ASEP in \[21\], various exact results for exclusion processes have been achieved via the MPA; see for example \[17\] and references therein. Since the method is now well known, we will skip a detailed presentation of the formalism and even omit the proof that the particular version presented here correctly determines the stationary state.

The MPA expresses the probability of any configuration in the stationary state of the AHR model, up to an overall normalization, as a trace of a product of certain matrices. Thus, for example, the probability $P$ of the configuration $+ - 00+$ can be written in the form

$$P(+) = Z^{-1} \text{Tr}(DEAAD).$$

Here $Z$ is an ensemble-dependent normalization constant which will be discussed shortly. The matrices $D$, $E$ and $A$ are assigned to the local states $+$, $-$ and $0$, respectively, and are required to satisfy the following algebraic conditions, which guarantee stationarity of the resulting state:

$$DE - qED = \zeta(D + E),$$

$$\alpha DA = \zeta A,$$

$$\alpha AE = \zeta A. \quad (2.1)$$

Here the number $\zeta$ is arbitrary; a natural choice, which we adopt from now on, is

$$\zeta = 1 - q. \quad (2.2)$$

The conditions (2.1) are closely related to those for the matrices of the MPA for the partially asymmetric simple exclusion processes \[17–19\].

It is convenient to introduce the new parameter

$$a = -1 + \frac{1 - q}{\alpha}. \quad (2.3)$$

In terms of $a$, explicit representations for the matrices $D$, $E$ and $A$ which satisfy (2.1) are given by

$$D = \begin{bmatrix} 1 + a & \sqrt{c_1} & 0 & 0 & \cdots \\ 0 & 1 + aq & \sqrt{c_2} & 0 & \cdots \\ 0 & 0 & 1 + aq^2 & \sqrt{c_3} & \cdots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix},$$

$$E = D^T,$$

and

$$A = |0\rangle\langle 0|, \quad (2.4)$$
where the superscript $T$ indicates the transpose,

$$c_n = (1 - q^n)(1 - a^2q^{n-1}),$$  

\(0| = [1 \ 0 \ 0 \ldots ]\), and \(|0\rangle = \langle 0| T\).

Recall that we take \(0 \leq q < 1\), and certainly \(a > -1\). Thus if \(a < 1\) then \(c_n\) is positive for any \(n \geq 1\), and the roots in (2.4) are real. If \(a \geq 1\) then the roots may be imaginary; moreover, \(c_n\) can vanish for special values of \(a\) and \(n\), leading to finite dimensional representations. The case \(a \geq 1\) requires special treatment in other ways, which we will mention briefly in section 3. In the future, unless special mention is made, we assume that \(-1 < a < 1\); this is the interesting case since the transition between the mixed and disordered regime occurs in this region (see Table 1 of \[15\]; our results below show that this transition in fact occurs for \(a < 0\)).

Since the matrices in (2.4) are infinite dimensional, it is not a priori clear that the trace of an arbitrary product of these matrices exists. However, \(A\) is a projector of rank one, so that the trace of any product of these matrices will exist as long as there is at least one \(A\) matrix in the product or, equivalently, as long as there is at least one hole in the corresponding configuration. We will consider here only such well defined traces since, as mentioned in the introduction, when there are no holes the model has a trivial steady state.

For the CE, in which \(N_+\) are specified, the normalization constant \(Z_{CE}^{CE}(N_+, N_-)\) is the sum of traces of matrix products over all configurations which respect the given \(N_+\) and \(N_-\). This ensemble is in many ways the natural one; Monte Carlo simulations for example, are usually done in the CE. However, it seems difficult to compute \(Z_{CE}^{CE}(N_+, N_-)\). It is easier to analyze the model in a superposition of CE’s, that is, in an appropriately defined GCE. There is a certain ambiguity in the definition of such an ensemble, but a standard method has emerged \[8,15\]. In the AHR model it would be natural to introduce different fugacities \(\xi_\pm\) for the two types of particles, but since we are interested in the case of equal densities, we set \(\xi_+ = \xi_- = \xi\). Thus we take the probability of a configuration \(\tau_1 \tau_2 \ldots \tau_L\), where \(\tau_j = +, -\) or 0 for \(j = 1, 2, \ldots , L\), to be

$$P^{GCE}(\tau_1, \tau_2, \ldots , \tau_L) = \frac{1}{Z_L(\xi)} \text{Tr} \prod_{n=1}^{L} \left[ \delta_{\tau_n} + \xi D + \delta_{\tau_n} - \xi E + \delta_{\tau_n} 0 A \right].$$  

(2.6)

Now the normalization constant \(Z_L(\xi) = Z_L^{GCE}(\xi)\) is a sum over traces of matrix products for all configurations of size \(L\) which have at least one hole, that is,

$$Z_L(\xi) = \text{Tr'} G^L$$  

(2.7)

with

$$G = A + \xi C$$  

(2.8)

where

$$C = D + E.$$  

(2.9)
Here the prime in $\text{Tr}'$ indicates a sum over all terms with at least one $A$. A more detailed discussion of the relationship between the CE and the GCE will be given in section 5.

The current $J_+$ of $+$ particles in the GCE is defined as the average flux of $+$ particles through a given bond. It is the same as the current $J_-$ of $-$ particles, defined similarly. The current $J = J_+ = J_-$ and the density $\rho = \rho_+ = \rho_-$ are easily seen to be given by

$$J_L(\xi) = (1 - q)\xi \frac{Z_{L-1}(\xi)}{Z_L(\xi)},$$

$$\rho_L(\xi) = \frac{\xi}{2L} \frac{\partial}{\partial \xi} \ln Z_L(\xi),$$

where the subscript $L$ indicates the system size. As pointed out in the introduction, we are interested in the infinite volume limits $J(\xi) = \lim_{L \to \infty} J_L(\xi)$ and $\rho(\xi) = \lim_{L \to \infty} \rho_L(\xi)$ of these quantities because a phase transition between the mixed and the disordered regime should manifest itself as non-analyticity in $J$ as a function of $\rho$. $J(\xi)$ and $\rho(\xi)$ will be computed in the next section.

### 3 Exact Results in the Thermodynamic Limit

Instead of considering $Z_L(\xi)$ directly, we introduce the generating function

$$\Theta(\lambda, \xi) = \sum_{L=1}^{\infty} \lambda^{L-1} Z_L(\xi).$$

This sum can be explicitly evaluated as follows. First we rewrite $Z_L(\xi)$ as a summation of the terms with the condition that the left-most hole is at site $j + 1$:

$$Z_L(\xi) = \sum_{j=0}^{L-1} \text{Tr}(\xi C)^j A G^{L-j-1} = \sum_{j=0}^{L-1} \langle 0 | G^{L-j-1} (\xi C)^j | 0 \rangle,$$

where we used the cyclicity of trace and the explicit representation of $A = |0\rangle\langle 0|$. Hence the generating function $\Theta(\lambda, \xi)$ is rewritten as

$$\Theta(\lambda, \xi) = \sum_{j,k=0}^{\infty} \langle 0 | (\lambda G)^k (\lambda \xi C)^j | 0 \rangle.$$

Second we expand $G^k$ as

$$G^k = \sum_{r\geq0} \sum_{j_0, j_r \geq 0} \sum_{j_1, m_1, \ldots, j_{r-1}, m_{r-1} \geq 0} \sum_{j_0 + m_1 + \cdots + m_{r-1} + j_r = k} (\xi C)^{j_0} A^{m_1} (\xi C)^{j_1} \cdots A^{m_r} (\xi C)^{j_r}.$$
If we observe that $A^m = A$ and define
\[
\chi(x) = \sum_{n=0}^{\infty} \frac{1}{x^{n+1}} \langle 0 | C^n | 0 \rangle = \langle 0 | \frac{1}{x - C} | 0 \rangle, \tag{3.5}
\]
so that
\[
\sum_{n=0}^{\infty} (\xi \lambda)^n \langle 0 | C^n | 0 \rangle = \frac{1}{\xi \lambda} \chi \left( \frac{1}{\xi \lambda} \right), \quad \sum_{n=0}^{\infty} (n + 1)(\xi \lambda)^n \langle 0 | C^n | 0 \rangle = \frac{1}{\xi} \frac{d}{d\lambda} \chi \left( \frac{1}{\xi \lambda} \right), \tag{3.6}
\]
then after some computation we obtain
\[
\Theta(\lambda, \xi) = \frac{d}{d\lambda} \chi \left( \frac{1}{\lambda \xi} \right). \tag{3.7}
\]

Finally it turns out that the function $\chi(x)$ has been known in mathematics literature [22]. This is related to the fact that the matrix $C$ is essentially the Jacobi matrix associated with certain $q$-orthogonal polynomials, called Al-Salam-Chihara polynomials [23] (and regarded as a special case of the Askey-Wilson polynomials [24]); see [17] for an explanation of this connection. For example, from [22], equation (3.21), it follows that
\[
\chi(x) = f(y(x)) \tag{3.8}
\]
with
\[
f(y) = y \frac{(q y^2; q)_{\infty} (q; q)_{\infty}}{(ay; q)_{\infty}^2} \sum_{n=0}^{\infty} \frac{(ay; q)_n^2}{(q y^2; q)_n (q; q)_n} q^n, \tag{3.9}
\]
\[
y(x) = \frac{x - 2 - \sqrt{x^2 - 4x}}{2}, \tag{3.10}
\]
where $(z; q)_n$ and $(z; q)_{\infty}$ are defined as
\[
(z; q)_n = \begin{cases} 
1, & \text{if } n = 0, \\
(1 - z)(1 - zq)(1 - zq^2) \cdots (1 - zq^{n-1}), & \text{if } n > 0,
\end{cases} \tag{3.11}
\]
\[
(z; q)_{\infty} = \prod_{n=0}^{\infty} (1 - zq^n). \tag{3.12}
\]

If we introduce the basic hypergeometric function [16]
\[
_2\phi_1 \left[ \begin{array}{c} a_1, a_2 \\ b \end{array} ; q, z \right] = \sum_{n=0}^{\infty} \frac{(a_1; q)_n (a_2; q)_n}{(b; q)_n (q; q)_n} z^n, \tag{3.13}
\]
\( (3.9) \) is rewritten as
\[
f(y) = \frac{(q y^2; q)_\infty (q; q)_\infty}{(a y; q)_\infty^2} 2\phi_1 \left[ \frac{a y, a y}{q y^2; q, q} \right].
\] (3.14)

This is the explicit expression of the generating function \( \Theta(\lambda, \xi) \).

Next we are interested in the asymptotic behavior of \( Z_L(\xi) \) when \( L \to \infty \). This is determined by the singularity closest to the origin of the generating function \( \Theta(\lambda, \xi) \) as a function of \( \lambda \). We do not demonstrate this fact here; for a thorough discussion see Appendix A of [12]. From the expression \( (3.7) \), we see that there are two possible sources of singularities in \( \Theta(\lambda, \xi) \): a singularity of the function \( \chi \left( \frac{1}{\lambda \xi} \right) \) (the differentiation in the numerator does not change the position of any singularities) and a zero of the denominator. As we will see, the singularity which is closest to the origin is always of the latter type, for the region of the parameter space of interest here.

First we consider the singularities of \( \chi \left( \frac{1}{\lambda \xi} \right) \). From \( (3.10) \) it follows that \( y(1/u) \) is analytic at \( u = 0 \), that the singularity closest to the origin is the square root singularity at \( u = 1/4 \), and that \( |y(1/u)| < 1 \) for \( |u| < 1/4 \). Moreover, from \( (3.9) \), the singularity of \( f(y) \) closest to the origin is a simple pole at \( y = 1/a \). Thus if \( \lambda_0(\xi) \) denotes the singularity of \( \chi \left( \frac{1}{\lambda \xi} \right) \) closest to the origin, then (i) \( \lambda_0(\xi) = 1/(4\xi) \) is a square root singularity if \( a < 1 \) and (ii) \( \lambda_0(\xi) = a/[(a+1)^2\xi] \) is a simple pole if \( a > 1 \). In what follows we restrict our detailed analysis to the case \( a < 1 \). (See remarks following \( (2.3) \); the analysis of \( a > 1 \) is similar.)

In order to discuss the zeros of the denominator of \( (3.7) \) we make the following assumption:

**If \( 0 \leq q < 1 \) then the function \( f \) satisfies \( f'(y) > 0 \) for \( 0 \leq y \leq 1 \).** (3.15)

This assumption is key for our analysis; we have considerable evidence for its truth, which we will discuss shortly, but at the moment no proof. From \( (3.8) \), \( (3.10) \), and \( (3.13) \) it follows that, when \( \xi \) is positive, the function \( \chi \left( \frac{1}{\lambda \xi} \right) \) increases monotonically from 0 to \( f(1) \) as \( \lambda \) increases from 0 to \( \lambda_0(\xi) \). Thus if \( \xi \) satisfies \( 0 \leq \xi \leq \xi_{\text{max}} \), where \( \xi_{\text{max}} = f(1) \), the equation
\[
\chi \left( \frac{1}{\lambda \xi} \right) = \xi
\] (3.16)

has a unique solution \( \lambda(\xi) \) in the interval \([0, \lambda_0(\xi)]\), and the denominator of \( (3.7) \) vanishes at this point. Since \( \lambda(\xi) \) is smaller than \( \lambda_0(\xi) \), this is the singularity of the function \( \Theta(\lambda, \xi) \) which is closest to the origin when \( 0 \leq \xi \leq \xi_{\text{max}} \). This singularity is a simple pole, so that \( Z_L(\xi) \) behaves asymptotically \( (L \to \infty) \) as
\[
Z_L(\xi) \simeq \text{const.} \left[ \frac{1}{\lambda(\xi)} \right]^L
\] (3.17)
Thus from (2.10) and (2.11),

\[
J(\xi) = \lim_{L \to \infty} J_L(\xi) = (1 - q)\xi\lambda(\xi), \quad (3.18)
\]

\[
\rho(\xi) = \lim_{L \to \infty} \rho_L(\xi) = -\frac{\xi}{2\partial\xi}\ln\lambda(\xi). \quad (3.19)
\]

These expressions can be simplified somewhat because the function \(y(x)\) is explicitly invertible. If we denote the inverse function of \(f(y)\) for \(0 \leq y \leq 1\) by \(g(\xi)\),

\[
\xi = f(y) \leftrightarrow y = f^{-1}(\xi) = g(\xi) \quad \text{for} \quad 0 \leq \xi \leq \xi_{\text{max}}, \quad 0 \leq y \leq 1,
\]

then the equation (3.16) can be rewritten as

\[
\lambda(\xi) = \frac{1}{\xi(1 + g(\xi))^2}. \quad (3.20)
\]

Combining the above results, we find

\[
J(\xi) = (1 - q)\frac{g(\xi)}{(1 + g(\xi))^2}, \quad (3.21)
\]

\[
\rho(\xi) = \frac{1}{2} \left[ 1 - \frac{\xi(1 - g(\xi))g'(\xi)}{(1 + g(\xi))g(\xi)} \right]. \quad (3.22)
\]

From (3.15) and (3.21) it follows that \(g(\xi)\) increases monotonically from 0 to 1 as \(\xi\) increases from 0 to \(\xi_{\text{max}}\) and, since \(g'(\xi) = 1/f'(g(\xi))\), that \(0 < g'(\xi) < \infty\) in this region. Then (3.22) and (3.23) imply that \(J\) and \(\rho\) are analytic functions of \(\xi\) throughout the range \(0 < \xi < \xi_{\text{max}}\), and that as \(\xi\) increases from 0 to \(\xi_{\text{max}}\), \(J(\xi)\) increases monotonically from 0 to \((1 - q)/4\) and \(\rho(\xi)\) increases from 0 to 1/2. We expect also, and will assume in what follows, that \(\rho(\xi)\) is a monotonic function throughout the range \(0 \leq \xi \leq \xi_{\text{max}}\). It follows that we may invert the function \(\rho(\xi)\) as \(\xi(\rho)\) and thus obtain an analytic function \(J(\rho) = J(\xi(\rho))\) defined for \(0 \leq \rho \leq 1/2\). This is the indication that there is no mixed/disordered phase transition in the GCE.

Note that for this argument it is important that \(f'(y)\) be strictly positive not only for \(0 \leq y < 1\) but also for \(y = 1\) (and hence \(g'(\xi)\) finite not only for \(0 \leq \xi < \xi_{\text{max}}\) but also for \(\xi = \xi_{\text{max}}\)); this guarantees the convergence of \(\rho(\xi)\) in (3.22) to 1/2 as \(\xi \to \xi_{\text{max}}\).

To obtain \(J(\rho)\) we must first invert the function \(f(y)\) to obtain \(g(\xi)\), then invert the function \(\rho(\xi)\) to obtain the fugacity as a function of the density. It is not possible to carry out these inversions explicitly in general, and we must use numerical methods to obtain \(J(\rho)\). But there are special cases where one or both of the inversions can be done explicitly. Let us study these cases first.

**Case 1.** \(q = 0\). For this case, the formula for \(f(y)\) in (3.9) is greatly simplified since 

\[
(z;0)_n = (z;0)_\infty = 1 - z \quad \text{and the only } n = 0 \text{ term in the infinite series of (3.9) remains.}
\]
We find
\[ f(y) = \frac{y}{(1 - ay)^2}, \quad (3.24) \]
\[ f'(y) = \frac{1 + ay}{(1 - ay)^3}. \quad (3.25) \]

Notice that the assumption \([3.15]\) holds in this case, since \(a > -1\). The function \(f(y)\) is invertible, and
\[ g(\xi) = 1 + 2a\xi - \sqrt{1 + 4a\xi}. \quad (3.26) \]

The explicit formulae for \(J(\xi)\) and \(\rho(\xi)\) are then given by
\[ J(\xi) = \frac{2a^2\xi}{1 + a^2 + 2a(1 + a)^2\xi - (1 - a^2)\sqrt{1 + 4a\xi}}, \quad (3.27) \]
\[ \rho(\xi) = \frac{a(1 + a)\xi[\sqrt{1 + 4a\xi} - (1 - a)]}{\sqrt{1 + 4a\xi}[1 + a^2 + 2a(1 + a)^2\xi - (1 - a^2)\sqrt{1 + 4a\xi}]} \quad (3.28) \]

These formulae are further simplified when \(a = 0\) (as pointed out in the introduction, setting \(a = q = 0\) reduces the AHR model to the two-species ASEP studied in \([8]\)). Now \(f(y) = y, g(\xi) = \xi,\), and
\[ J(\xi) = \frac{\xi}{(1 + \xi)^2}, \quad (3.29) \]
\[ \rho(\xi) = \frac{\xi}{1 + \xi}. \quad (3.30) \]

From the easy inversion of \([3.30]\) we obtain the known current density relation
\[ J = \rho(1 - \rho). \quad (3.31) \]

**Case 2.** \(a = -1\). This case corresponds to taking the limit \(q \to 1\) with \(\alpha\) fixed, and is thus strictly speaking outside our parameter region \(0 \leq q < 1\), but it is nevertheless of interest. Moreover, it will play the role of zeroth-order approximation in the analysis of the next section; for this reason, the functions for this special case will be distinguished by the superscript \((0)\) in the following. Using the formula for \(2\phi_1 [16] \),
\[ 2\phi_1 \left[ \frac{a_1, a_2}{b}; q, \frac{b}{a_1a_2} \right] = \frac{(b/a_1; q)_\infty(b/a_2; q)_\infty}{(b; q)_\infty(b/a_1a_2; q)_\infty}, \quad (3.32) \]
we find
\[ f^{(0)}(y) = \frac{y}{(1 + y)^2}, \quad (3.33) \]
\[ \frac{\partial}{\partial y} f^{(0)}(y) = \frac{1 - y}{(1 + y)^3}. \quad (3.34) \]

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Assumption (3.15) is not strictly satisfied, since $\partial f^{(0)}(y)/\partial y = 0$ for $y = 1$, but $f(y)$ is strictly monotone for $0 \leq y \leq 1$ so that the derivation of the asymptotic form (3.17) is still valid. Note that (3.33) and (3.34) are independent of $q$ and hence may be obtained by setting $a = -1$ in (3.26) and (3.27). Hence the explicit formulae for $g(\xi), J(\xi)$ are obtained by simply taking $a = -1$ in (3.26) and (3.27):

\[ g^{(0)}(\xi) = 1 - 2\xi - \sqrt{1 - 4\xi}, \]  
\[ J^{(0)}(\xi) = \xi. \]  

As for $\rho(\xi)$, we have $\rho^{(0)}(\xi) = 0$ for $0 \leq \xi < \xi_{\text{max}} = 1/4$, while $\rho^{(0)}(1/4)$ is not well specified. Thus we cannot achieve nonzero density values by any specification of the fugacity: the $q \to 1$ limit is a very singular limit for the density-fugacity relation.

We now turn to the question of the validity of the key assumption (3.15). We believe, although we have not proved, that (3.15) holds for all $a, q$ satisfying $-1 < a < 1$ and $0 \leq q < 1$. This belief is based on several pieces of evidence. We have evaluated the functions $f(y)$ and $f'(y)$ numerically for various values of $a, q,$ and $y$ and have always found that $f'(y) > 0$ for $0 \leq y \leq 1$ (such evaluations are easily carried out to arbitrarily high accuracy from the formula (3.9)). We do observe, however, that for $q$ and $y$ close to 1 the value of $f'(y)$ is very small; for instance, $f'(1)$ is of order $10^{-36}$ when $q = 0.9$ and $\alpha = 1$. This phenomenon will play a key role in the analysis of section 4. Note also that it follows from the considerations of the special cases above that (3.15) holds when $q = 0$, and that when $a = -1$ (recall that this corresponds to a limit $q \to 1$), $f'(y) > 0$ when $0 \leq y < 1$; this suggests that $f'(y) > 0$ except at the corner $q = y = 1$ of the region of interest. Moreover, we will show in the next section that $f'(1) > 0$ when $\alpha = 1$ (i.e., $q = -a$). This is a weaker statement than (3.15) but, since $f(y)$ is expected to be a monotonically decreasing function, is a strong analytical indication that (3.15) holds when $q = -a$.

4 Two Distinct Regimes without Non-analyticity

In the previous section we argued that, even in infinite volume, the current is an analytic function of the density throughout the mixed/disordered phase. On the other hand, it is clear from inspection of the $J$-$\rho$ diagram in the thermodynamic limit that, for large values of $q$, the derivative of $J(\rho)$ does change rapidly—in fact, extraordinarily rapidly—as $\rho$ passes through some critical value $\rho_c$. For example, when $q = -a = 0.9$, there is a change of order one in $J'(\rho)$ arising from a change of order $10^{-24}$ in $\rho$ (see Fig. 2). In this section, we explain how this behavior arises: it is associated with the very small values of $f'(1)$ occurring when $q$ is near 1, which lead to rather peculiar behavior in the density-fugacity relation (3.23).

In Fig. 3, we graph the functions $J(\xi)$ and $\rho(\xi)$ of (3.22), (3.23) for $\alpha = 1$ and several values of $q$. Note that, although the function $J(\xi)$ remains quite smooth as $q$ increases, and
indeed even for \( q = 1 \), the function \( \rho(\xi) \) develops an apparently sharp corner or kink, even for values of \( q \) about 0.75; this kink corresponds to the kink in the \( J-\rho \) curve at \( \rho_c \). Here we give an approximate analysis of this behavior under the assumption that \( q \) is reasonably near to 1 and that \( f'(1) \) is very small.

We first analyze the region \( \rho < \rho_c \). Using the formula (see [16])

\[
2 \phi_1 \left[ \begin{array}{c} a_1, a_2 \\ b \end{array} ; q, z \right] = \frac{(a_2; q) \infty (a_1 z; q) \infty}{(b; q) \infty (z; q) \infty} 2 \phi_1 \left[ \begin{array}{c} b/a_2, z \\ a_1 z \end{array} ; q, a_2 \right],
\]

we obtain an alternate expression for \( f(y) \):

\[
f(y) = \frac{y}{1 - ay} \sum_{n=0}^{\infty} \frac{(a^{-1} q y; q)_n}{(a q y; q)_n} (ay)^n.
\]  

(4.2)

Since we are interested in values of \( q \) close to 1 we set \( q = 1 - \epsilon \), where \( \epsilon (> 0) \) is assumed to be small, and expand in \( \epsilon \), denoting quantities accurate to order \( k \) by a corresponding superscript (e.g. \( f^{(k)} \)). The 0th order was analyzed in the previous section; here we will carry out the expansion to first order. By a straight-forward computation we obtain

\[
f^{(1)}(y) = \frac{y}{(1+y)^2} \left[ 1 + \frac{2y}{\alpha (1+y)^2} \epsilon \right] = f^{(0)}(y) \left[ 1 + \frac{2 f^{(0)}(y)}{\alpha} \epsilon \right].
\]  

(4.3)

As \( y \) increases from zero to one, \( f^{(1)}(y) \) increases monotonically from zero to \( \xi^{(1)}_{\text{max}} = 1/4 + \epsilon/(8 \alpha) \). The function \( f^{(1)}(y) \) is invertible, with inverse

\[
g^{(1)}(\xi) = g^{(0)}(X(\xi)) = \frac{1 - 2X(\xi) - \sqrt{1 - 4X(\xi)}}{2X(\xi)},
\]  

(4.4)

where

\[
X(\xi) = \frac{\alpha}{4 \epsilon} \left( \sqrt{1 + \frac{8 \epsilon \xi}{\alpha}} - 1 \right),
\]  

(4.5)

for \( 0 \leq \xi \leq \xi^{(1)}_{\text{max}} \). Then the density-fugacity relation (3.23) becomes

\[
\rho(\xi) = \frac{1}{2} \left[ 1 - \frac{\xi d X(\xi)}{X(\xi)} \right] + O(\epsilon^2),
\]  

(4.6)

so that to first order in \( \epsilon \) the density is

\[
\rho^{(1)}(\xi) = \frac{\epsilon \xi}{\alpha}.
\]  

(4.7)

Comparing these results with the curve for \( q = 0.75 \) in Fig. 3, we realize that (4.6) gives the behavior of the density-fugacity relation up to the kink; since this region includes \( \xi = 0 \)
(or $\rho = 0$), it corresponds to the disordered regime. As the fugacity $\xi$ increases from zero to $\xi_{\text{max}}^{(1)}$, the density $\rho^{(1)}$ increases linearly from zero to $\epsilon/(4\alpha)$, so that this value may be identified, up to first order, with the density $\rho_c$:

$$\rho^{(1)}_c = \frac{\epsilon}{4\alpha}. \quad \text{(4.8)}$$

Note that under this analysis there is no value of $\xi$ which gives rise to a density $\rho$ in the interval $(\rho_c, \frac{1}{2}]$. This is because our approximation of $f(y)$ by $f^{(1)}(y)$ lacks an important property of the original $f(y)$: the derivative of $f^{(1)}$ becomes zero at $y = 1$, whereas our basic assumption (3.15) is that $f'(1) > 0$. In fact, it appears that $f''(1)$ vanishes to all orders in the perturbation expansion in $\epsilon$; this is shown below (see (4.24)) in the case $q = -a$.

We now analyze the region $\rho_c < \rho \leq \frac{1}{2}$ under the assumption that $f'(1)$ is positive but very small. We will also assume (as is supported by numerical evaluations) that $f''(1)$ is negative and of order unity. Under these assumptions, and recalling that $f(1) = \xi_{\text{max}}$, we may approximate $f(y)$ near $y = 1$ as

$$f(y) \simeq f^*(y) = \xi_{\text{max}} - B((1 + \delta - y)^2 - \delta^2), \quad \text{(4.9)}$$

where $B = -f''(1)$ and $\delta = -f'(1)/f''(1)$; that is, $f(y)$ will have a quadratic maximum at approximately $1 + \delta$, where $\delta$ is very small. The function $f^*(y)$ has inverse

$$g^*(\xi) = 1 + \delta - \sqrt{\frac{\xi_{\text{max}} - \xi}{B}} + \delta^2 = 1 + \delta - \delta \sqrt{\eta + 1}, \quad \text{(4.10)}$$

where for $\xi \simeq \xi_{\text{max}}$, it is convenient to introduce the scaled variable $\eta$ defined by

$$\xi_{\text{max}} - \xi = \eta \delta^2. \quad \text{(4.11)}$$

The density-fugacity relation (3.23) then becomes $\rho(\xi) \simeq \rho^*(\xi)$, where

$$\rho^*(\xi) = \frac{1}{2} \left[ 1 - \frac{\xi_{\text{max}}}{4B} \sqrt{\eta + 1} - \frac{1}{\sqrt{\eta + 1}} \right], \quad \text{(4.12)}$$

so that as $\eta$ goes infinity, $\rho^*(\xi)$ approaches

$$\rho^*_c = \frac{1}{2} \left[ 1 - \frac{\xi_{\text{max}}}{4B} \right]. \quad \text{(4.13)}$$

Thus here the critical density $\rho_c$ arises as the minimum value of the density which can be described by (4.12). Clearly (4.12) describes the density-fugacity relation in the mixed regime, that is, for $\rho > \rho_c$. When $q = 0.75$, for example, this corresponds to the nearly vertical line shown in Fig. 3. The value $\rho_c$ of (4.13) is an extremely accurate value for the “critical density” between the mixed and disordered regimes when $q$ is close to one; this is the value used in plotting Fig. 2 and thus in the case $q = -a = 0.9$ is accurate to about $10^{-24}$.
Note that (4.3) implies that to first order in $\epsilon$, $B = 1/16 + \epsilon/(16\alpha)$; recalling that $\xi_{\text{max}}^{(1)} = 1/4 + \epsilon/(8\alpha)$, we see that (4.13) reduces to (4.8) in first order. In [15] the critical value of $\rho$ was estimated, on the basis of extrapolation of finite size data, to be (in our notation) $(1 - q)/(4\alpha - 2(1 - q))$; this value agrees with (4.13) to first order in $\epsilon$.

The key point for the above analysis, as we have emphasized, is that $f'(1)$ is “very small” over a range of $q$ values close, but not necessarily very close, to 1. We can throw some additional light on this phenomenon because, in the special case $\alpha = 1$, it is possible to compute $f'(1)$ exactly. When $\alpha = 1$, i.e., when $a = -q$, the expression of $f(y)$ in (4.2) can be further simplified as

$$f(y) = \frac{1}{1 - q} \left[ (1 + y)^2 \sum_{n=0}^{\infty} \frac{(-qy)^n}{1 + yq^n} - 1 \right],$$

so that

$$f'(1) = \frac{4}{1 - q} \left[ \sum_{n=0}^{\infty} \frac{(-q)^n}{(1 + q^n)^2} + \sum_{n=1}^{\infty} \frac{n(-q)^n}{1 + q^n} \right].$$

The sums in (4.13) can be evaluated explicitly, using the formulae [16]

$$\sum_{n=1}^{\infty} \frac{(-q)^n}{(1 + q^n)^2} = \sum_{n=1}^{\infty} \frac{n(-q)^n}{1 + q^n} = \frac{1}{8} \left( \left[ \frac{(q; q)_\infty}{(-q; q)_\infty} \right]^4 - 1 \right).$$

This leads to

$$f'(1) = \frac{1}{1 - q} \left[ \frac{(q; q)_\infty}{(-q; q)_\infty} \right]^4.$$  (4.17)

This expression is valid for any value of $q$ satisfying $0 \leq q < 1$, and is clearly positive. The behavior of $f'(1)$ as a function of $q$ is shown in Fig. 4.

Now we consider the asymptotic behavior of $f'(1)$ as $\epsilon = 1 - q$ becomes small. Setting $q = e^{-\pi^2 t}$, we find

$$\frac{(q; q)_\infty}{(-q; q)_\infty} = \prod_{n=1}^{\infty} \frac{1 - q^n}{1 + q^n} = \sum_{n=-\infty}^{\infty} (-)^n e^{-\pi^2 n^2 t} = \vartheta_0(0, i\pi t).$$

Here $\vartheta_0(x, \tau)$ is an elliptic theta function defined by

$$\vartheta_0(x, \tau) = \sum_{n=-\infty}^{\infty} (-)^n e^{i\pi nx^2 + 2\pi i nx}.  \quad (4.19)$$

Applying Jacobi’s imaginary transformation,

$$\vartheta_0(x, \tau) = \frac{1}{\sqrt{-i\tau}} e^{-i\pi x^2/\tau} \vartheta_2 \left( \frac{x}{\tau}, -\frac{1}{\tau} \right).  \quad (4.20)$$
with
\[ \vartheta_2(x, \tau) = \sum_{n = -\infty}^{\infty} e^{i\pi \tau(n-1/2)^2 + i\pi x(2n-1)}, \] (4.21)
we obtain
\[ \frac{(q; q)_\infty}{(-q; q)_\infty} = \frac{1}{\sqrt{\pi t}} \sum_{n = -\infty}^{\infty} e^{-(n-1/2)^2/t}. \] (4.22)
(These formula involving theta functions are easily obtained from, for example, Chapter 21 of [25].) Now it is easy to read off the asymptotic behavior as \( q \) approaches 1. The leading contributions come from the \( n = 0 \) and \( n = 1 \) terms in (4.22). Since \( t \approx \epsilon / \pi^2 + \epsilon^2 / (2\pi^2) \), we find
\[ \frac{(q; q)_\infty}{(-q; q)_\infty} \approx \frac{2}{\sqrt{\pi t}} e^{-1/4} \approx 2 \sqrt{\frac{\pi}{\epsilon}} \pi e^{-\pi^2/4\epsilon}. \] (4.23)
Finally we obtain the asymptotic expression for \( f'(1) \):
\[ f'(1) \approx \frac{2^4 \pi^2}{e^3} e^{\pi^2 e^{-\pi^2/\epsilon}}. \] (4.24)
Using (3.23), it is also possible to obtain the asymptotic expression for \( \delta \):
\[ \delta = \frac{f'(1)}{2B} \approx \frac{2^7 \pi^2}{e^3} e^{\pi^2 e^{-\pi^2/\epsilon}}. \] (4.25)

5 Density Fluctuations and the Canonical Ensemble

In the previous two sections, we have studied the current in the thermodynamic limit in the framework of a GCE. Our analysis strongly suggests that there is no phase transition between the mixed and disordered regimes in the GCE. In this section we argue that in the thermodynamic limit, the current in the GCE and the CE are the same, that is, that the current \( J(\rho) \) discussed in Section 3 and 4 is the same as the infinite volume limit of the current in the CE ensemble with density \( \rho \). This implies that the lack of a phase transition in the GCE discussed above also holds for the CE. The argument also sheds some light on the structure of the infinite volume state of the model in the mixed/disordered regime.

In finite volume, the GCE is a superposition of canonical ensembles: contributions come from all values of the densities, with weights which are determined by the fugacity \( \xi \). The total mean density of particles (both + and −) is \( 2\rho_L(\xi) \), where \( \rho_L(\xi) \) is given by formula (2.11). The fluctuations in the total density can be expressed similarly (ideally we should discuss fluctuations in the density of each species, but that seems more difficult). If we write \( N = N_+ + N_- \) and introduce the quantity
\[ F_L(\xi) = \frac{1}{L} \left( \langle N^2 \rangle_L - \langle N \rangle_L^2 \right) = \frac{1}{L} \left( \xi \frac{\partial}{\partial \xi} \right)^2 \ln Z_L(\xi), \] (5.1)
then the fluctuations in the total density are simply given by $F_L(\xi)/L$. Now if we take the thermodynamic limit in the GCE for some fixed $\xi$, then the mean total density $2\rho_L(\xi)$ is expected to have a well defined limiting value, $2\rho(\xi) = \lim_{L \to \infty} 2\rho_L(\xi)$. If we can show that the fluctuations in the total density go to zero in the thermodynamic limit, then we expect that in this limit only a single total density $2\rho(\xi)$ survives, and if we ignore the possibility of canceling fluctuations in the $+$ and $-$ densities then these densities will also be unique in the limit. Thus, in the thermodynamic limit, the GCE with fugacity $\xi$ is the same as a CE with $(+)$ or $(-)$ density $\rho(\xi)$. This corresponds to the usual GCE/CE equivalence for equilibrium systems away from a phase transition. For our model, of course, condensation of particles in the mixed regime suggests a possible phase transition, and we need an independent argument. It turns out that we can exactly calculate $F(\xi) = \lim_{L \to \infty} F_L(\xi)$ from (3.23):

$$F(\xi) = 2\xi \frac{\partial}{\partial \xi} \rho(\xi) = \frac{\xi}{g(\xi)^2[1 + g(\xi)]^2} \left( \xi(1 + 2g(\xi) - g(\xi)^2)g'(\xi)^2 \right.
\left. - \xi(1 - g(\xi)^2)g(\xi)g''(\xi) - (1 - g(\xi)^2)g(\xi)g'(\xi) \right).$$

(5.2)

Numerical values of this quantity can be very large. For instance, for $q = -a = 0.9$, we find that $F(\xi)$ is of order $10^{70}$ in the region $\rho > \rho_c$. However, the important point is that $F_L(\xi)$ has a finite value in the thermodynamic limit, so that the density fluctuations $F_L/L$ in the finite system vanish in the infinite system. As argued above, this suggests that our analysis in the previous two sections, of the behavior of $J(\rho)$ in the GCE, is valid for the CE as well.

It is also possible to estimate the length scale $R$ up to which particle condensation will be observed in Monte Carlo simulations. Let us write $\langle N^2 \rangle = \sum_{1 \leq i,j \leq L} \sigma_i \sigma_j$ in (5.1), where $\sigma_i = 1$ if there is a particle at site $i$ and $\sigma_i = 0$ otherwise. If we assume that the particle-particle correlation function decays exponentially with some characteristic length $R$, $\langle \sigma_i \sigma_j \rangle \sim e^{-|i-j|/R}$, then we see that $F_L \sim R$. Thus the correlation length can become huge; for instance, for the above case of $q = -a = 0.9$, $R$ would be of the order $10^{70}$. Therefore it is certainly not possible to observe the breakdown of the particle condensation with Monte Carlo simulations.

The discussion of this section also throws light on our assumption of section 3, that $\rho(\xi)$ is a strictly increasing function. Since $2\xi \partial \rho_L / \partial \xi = F_L$ is a fluctuation, $\partial \rho_L / \partial \xi$ must be positive, so that $\partial \rho / \partial \xi \geq 0$. Vanishing of $\partial \rho / \partial \xi$ could occur only with subnormal fluctuations in $N$ ($\lim_{L \to \infty} F_L = 0$), a scenario which is certainly unlikely and has been ruled out in certain equilibrium situations [26].

6 Concluding Remarks

In this article we have studied an exclusion process on a ring, originally introduced and investigated by Arndt et al [14,15]. Using the theory of $q$-orthogonal polynomials, we have obtained the exact expression of the current in the thermodynamic limit in the framework
of a grand canonical ensemble (GCE). Contrary to what is suggested by Monte Carlo simulations and finite volume calculations, we find no phase transition between the mixed and the disordered regime; specifically, the infinite volume current as a function of the density is analytic through the mixed/disordered phase. However, the derivative of the current can change rapidly over a very small (but finite) interval of $\rho$, especially if $q$ is close to 1.

Our analysis of the infinite volume current depends on a key assumption, inequality (3.15). Although this is unproved, we have strong evidence of its truth: it holds in the special case $q = 0$ (and essentially also the special case $a = -1$); it is supported by the analysis of section 4 for the case $q = -a$; and we have checked its validity for various parameter values by highly accurate numerical computations. However, the rigorous proof of (3.15) remains an outstanding problem. A second assumption, the positivity of $\rho'(\xi)$, is physically natural and is also supported by numerical calculation.

Most of our analysis was carried out in a GCE. The relation between the canonical and grand canonical ensembles in equilibrium statistical mechanics has been well studied, but we know of no general results for non-equilibrium situations. Here we have simply asked how far the results for our GCE (which itself represents a particular and perhaps non-canonical choice) are also valid for the CE. We have given a heuristic argument: exact calculations show that the density fluctuations in the GCE vanish in the thermodynamic limit, which suggests that, in this limit, the GCE for a given fugacity agrees with the CE for a certain corresponding density.

It is fascinating that in the relatively simple AHR model one already has a quite subtle transition between the disordered and the mixed regime. As discussed in section 5, computer simulations would need to be carried out up to lattice sizes of the order $10^{70}$ (when $q = -a = 0.9$) to see the breakdown of the particle condensation, so that this is certainly a phenomenon which one would not expect from the accessible finite size Monte Carlo data.

**Acknowledgment**

The authors would like to thank J. L. Lebowitz for fruitful discussions and comments. NR gratefully acknowledges a postdoctoral fellowship from the Deutsche Forschungsgemeinschaft and thanks Joel Lebowitz for hospitality at the Mathematics Department of Rutgers University and for support under NSF grant DMR 95--23266, and thanks DIMACS and its supporting agencies, the NSF under contract STC--91--19999 and the NJ Commission on Science and Technology, for support. TS thanks the continuous encouragement of M. Wadati. TS is a Research Fellow of the Japan Society for the Promotion of Science.
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Figure Captions

Fig. 1: Space time diagrams of the AHR model from Monte Carlo simulations. The horizontal axis represents the site number $j$ whereas the vertical axis represents time. The existence of a positive (resp. negative) particle is represented as a black (resp. gray) point. For all three figures, we set $L = 100$, $N_+ = N_- = 30$, $\alpha = 0.5$. The left-most figure corresponds to the pure phase ($p_R = 0.9, p_L = 1$). The figure in the middle corresponds to the mixed regime ($p_R = 1, p_L = 0.9$). The right-most figure corresponds to the disordered regime ($p_P = 1, p_L = 0$).

Fig. 2: The $J$-$\rho$ diagram for the case $\alpha = 1, q = 0.9$. The horizontal and vertical axes of the inset are $(\rho - \rho_c) \times 10^{24}$ and $(J/(1 - q) - 0.25) \times 10^{23}$ respectively. The function $J(\rho)$ is analytic, although its derivative changes very rapidly as $\rho$ passes $\rho_c$.

Fig. 3: The functions $J(\xi)$ and $\rho(\xi)$ when $\alpha = 1$. For $q = 0$, we have $J(\xi) = \xi/(1 + \xi)^2$ (3.29) and $\rho(\xi) = \xi/(1 + \xi)$ (3.30). For $q = 1$, we have $J(\xi) = \xi$ (3.36) and $\rho(\xi) = 0 (0 \leq \xi < 1/4)$. The function $J(\xi)$ for $0 < q < 1$ interpolates these two limiting cases smoothly. On the other hand, as $q$ increases from zero, there appear two distinct regions for $\rho(\xi)$. In particular, the $q \rightarrow 1$ limit appears to be singular.

Fig. 4: The behavior of $f'(1)$ as a function of $q$. We see that $f'(1)$ becomes extremely small as $q$ approaches one.
\[ \frac{J}{1-q} \]

Figure 2
Figure 3
Figure 4