Infinite particle reaction models and random walks in the positive orthant

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1 Infinite particle model

Initial conditions At time $t = 0$ on the real axis there is a random configuration of particles, consisting of (+)-particles and (−)-particles. (+)-particles and (−)-particles differ also by the type: denote $I_+ = \{1, 2, ..., K\}$ the set of types of (+)-particles, and $I_- = \{1, 2, ..., L\}$ - the set of types of (−)-particles. Let

$$0 < x_{1,k} = x_{1,k}(0) < ... < x_{j,k} = x_{j,k}(0) < ...$$

be the initial configuration of particles of type $k \in I_+$, and

$$\cdots < y_{j,i} = y_{j,i}(0) < \cdots < y_{1,i} = y_{1,i}(0) < 0$$

be the initial configuration of particles of type $i \in I_-$, where the first index is the number of the particle in the configuration, the second index is its type. Thus all (+)-particles are situated on R_+ and all (−)-particles on R_-. Distances between neighbor particles of the same type denote by

$$\begin{aligned} x_{j,k} - x_{j-1,k} &= u^{(+)}_{j,k}, \quad k \in I_+, \quad j = 1, 2, ... \\ y_{j-1,i} - y_{j,i} &= u^{(-)}_{j,i}, \quad i \in I_-, \quad j = 1, 2, ... \end{aligned}$$

where we put $x_{0,k} = y_{0,i} = 0$. The random configurations corresponding to the particles of different types are assumed to be independent. The random distances between neighbor particles of the same type are also assumed to be independent, and moreover identically distributed, that is random variables $u^{(-)}_{j,i}, u^{(+)}_{j,k}$ are independent and their distribution depends only on the upper and second lower indices. Our technical assumption is that all these distribution are absolutely continuous and have finite means. Denote $\mu^{(-)}_i = Eu^{(-)}_{j,i}$, $\rho^{(-)}_i = \left(\mu^{(-)}_i\right)^{-1}, i \in I_-$, $\mu^{(+)}_k = Eu^{(+)}_{j,k}$, $\rho^{(+)}_k = \left(\mu^{(+)}_k\right)^{-1}, k \in I_+$.

Dynamics We assume that all (+)-particles of the type $k \in I_+$ move in the left direction with the same constant speed $v^{(+)}_k$, where $v^{(+)}_1 < v^{(+)}_2 < ... < v^{(+)}_K < 0$. The (−)-particles of type $i \in I_-$ move in the right direction with the same constant speed $v^{(-)}_i$, where $v^{(-)}_1 > v^{(-)}_2 > ... > v^{(-)}_L > 0$. If at some time t a (+)-particle and a (−)-particle are at the same point (we

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call this a collision or annihilation event), then both disappear. Collisions between particles of different types is the only interaction, otherwise they do not see each other. Thus, for example, at time t the $j-$th particle of type $k \in I_+$ could be at the point

$$x_{j,k}(t) = x_{j,k} + v_k^{(+)} t$$

if it will not collide with some $(-)$-particle before time t.

We define the boundary $\beta(t)$ between plus and minus phases to be the coordinate of the last collision which occured at some time $t' \le t$. For $t = 0$ we put $\beta(0) = 0$. Thus the trajectories of the random process $\beta(t)$ are piecewise constant functions, we shall assume them continuous from the left. We shall prove the a.e. existence of the limit

$$W = \lim_{t\to\infty} \frac{\beta(t)}{t} \tag{1}$$

which we call the asymptotical speed of the boundary. However our main goal is explicit calculation of W.

Result For any pair (J_-, J_+) of subsets , $J_- \subseteq I_-, J_+ \subseteq I_+$, define the number

$$V(J_-, J_+) = \frac{\sum_{i\in J_-} v_i^{(-)} \rho_i^{(-)} + \sum_{k\in J_+} v_k^{(+)} \rho_k^{(+)}}{\sum_{i\in J_-} \rho_i^{(-)} + \sum_{k\in J_+} \rho_k^{(+)}}, \qquad V(I_-, I_+) = V$$

The following condition is assumed

$$\{V(J_-, J_+) : \ J_- \neq \varnothing, \ J_+ \neq \varnothing \} \cap \{v_1^{(-)}, ..., v_L^{(-)}, v_1^{(+)}, ..., v_K^{(+)}\} = \varnothing . \tag{2}$$

If the limit $W = \lim\limits_{t\to\infty} \dfrac{\beta(t)}{t}$ exists a.e., we call it the asymptotic speed of the boundary.

Theorem 1 *The asymptotic velocity of the boundary exists and is equal to*

$$W = V(\{1, ..., L_1\}, \{1, ..., K_1\})$$

where

$$L_1 = \arg\max_{l\in I_-} V(\{1, ..., l\}, I_+) = \max\left\{ l \in \{1, \dots, L\} : \ v_l^{(-)} > V(\{1, ..., l\}, I_+) \right\},$$

$$K_1 = \arg\min_{k\in I_+} V(I_-, \{1, ..., k\}) = \max\left\{ k \in \{1, \dots, K\} : \ v_k^{(+)} < V(I_-, \{1, ..., k\}) \right\}.$$

Now we will explain this result in more detail. It is always true that $v_K^{(+)} < 0 < v_L^{(-)}$ and there can be 3 possible ordering of the numbers $v_L^{(-)}, v_K^{(+)}, V$:

1. $v_K^{(+)} < V < v_L^{(-)}$. In this case

$$K_1 = K, \quad L_1 = L, \quad W = V$$

2. If $v_K^{(+)} > V$ then $V < 0$ and $K_1 < K, \quad L_1 = L$. Moreover

$$W = V(\{1, ..., L\}, \{1, ..., K_1\}) = \min_{k\in I_+} V(\{1, ..., L\}, \{1, ..., k\}) \ < \ V \ < \ 0$$

3. If $v_L^{(-)} < V$ then $V > 0$ and $K_1 = K, \quad L_1 < L$. Moreover

$$W = V(\{1, ..., L_1\}, I_+) = \max_{l\in I_-} V(\{1, ..., l\}, I_+) \ > \ V \ > 0$$

2 Random walks in R_+^N

One can consider the phase boundary as a special kind of server where the customers (particles) arrive in pairs of the same type and are immediately served. However the situation is more involved, than in standard queueing theory, because the server moves, and correlation between between its movement and arrivals is sufficently complicated. That is why this analogy does not help much. However we describe the crucial correspondence between random walks in R_+^N and the infinite particle problem defined above which allows to get the solution.

Denote $b_i^{(-)}(t)$ ($b_k^{(+)}(t)$) the coordinate of the extreme right (left), and still existing at time t, that is not annihilated at some time $t' \le t$, $(-)$-particle of type $i \in I_-$ ($(+)$-particle of type $k \in I_+$). Define the distances $d_{i,k}(t) = b_k^{(+)}(t) - b_i^{(-)}(t) \ge 0$, $i \in I_-, k \in I_+$. The trajectories of the random processes $b_i^{(-)}(t)$, $b_k^{(+)}(t)$, $d_{i,k}(t)$ are assumed left continuous, for any indices. Consider the random process $D(t) = (d_{i,k}(t), (i,k) \in I) \in R_+^N$, where $N = KL$. $D(t)$ is a Markov process, due to our assumptions concerning initial distribution.

Denote $\mathcal{D} \in R_+^N$ the state space of $D(t)$. Note that the distances $d_{i,k}(t)$, for any t, satisfy the following conservation laws

$$d_{i,k}(t) + d_{n,m}(t) = d_{i,m}(t) + d_{n,k}(t)$$

where $i \ne n$ and $k \ne m$. That is why the state space $\mathcal{D}$ can be given as the set of non-negative solutions of the system of $(L-1)(K-1)$ linear equations

$$d_{1,1} + d_{n,m} = d_{1,m} + d_{n,1}$$

where $n, m \ne 1$. It follows that the dimension of $\mathcal{D}$ equals $K + L - 1$. However it is convenient to speak about random walk in R_+^N, taking into account that only subset of dimension $K+L-1$ is visited by the random walk.

Now we describe the trajectories $D(t)$ in more detail. The coordinates $d_{i,k}(t)$ decrease linearly with the speeds $v_i^{(-)} - v_k^{(+)}$ correspondingly until one of the coordinates $d_{i,k}(t)$ becomes zero. Let $d_{i,k}(t_0) = 0$ at some time t_0. This means that $(-)$-particle of type i collided with $(+)$-particle of type k. Let them have numbers j and l correspondingly. Then the components of $D(t)$ become:

$$\begin{aligned} d_{i,k}(t_0+0) &= u_{j+1,i}^{(-)} + u_{l+1,k}^{(+)} \\ d_{i,m}(t_0+0) - d_{i,m}(t_0) &= u_{j+1,i}^{(-)}, \quad m \ne k \\ d_{n,k}(t_0+0) - d_{n,k}(t_0) &= u_{l+1,k}^{(+)}, \quad n \ne i \end{aligned}$$

and other components will not change at all, that is do not have jumps. Shortly, it can be summarized as follows. Let $d_{i,k}(t_0) = 0$, then for any n, m

$$d_{n,m}(t_0+0) - d_{n,m}(t_0) = \delta(n,i) u_{j+1,i}^{(-)} + \delta(m,k) u_{l+1,k}^{(+)}$$

where $\delta(n,i) = 1$ for $n = i$ and $\delta(n,i) = 0$ for $n \ne i$. Note that the increments of the coordinates $d_{n,m}(t_0+0) - d_{n,m}(t_0)$ at the jump time do not depend on the history of the process before time t_0, as the random variables. $u_{j,i}^{(-)}(u_{j,k}^{(+)})$ are independent and equally distributed for fixed type. Markov property follows from this.

Note however that this continuous time Markov process has singular transition probabilities (due to partly deterministic movement). This fact however does not prevent us from using

the techniques from [1] where random walks in Z_+^N were considered. Absolute continuity of the distributions of random variables $u_{j,i}^{(-)}$,$u_{j,k}^{(+)}$ garanties that the events when more than one coordinate of $D(t)$ become zero, have zero probability.

We call the process $D(t)$ ergodic, if there exists a neighborhood A of zero, such that the mean value $E\tau_x$ of the first hitting time τ_x of A from the point x is finite for any $x \in \mathcal{D}$. In our context we call the process $D(t)$ transient if it goes to infinity with probability 1. Condition (2), which excludes the set of parameters of zero measure, excludes null recurrent cases and complicated behavior of considered random walk as well.

Any collision of particles of the types $i \in I_-, k \in I_+$ is called a collision of type (i,k). Denote

$$\nu_{i,k}(T) = \#\{t : d_{i,k}(t) = 0, t \in [0,T]\}$$

-that is the number of collisions of type (i,k) on the time interval $[0,T]$. One can calculate the asymptotics of these numbers due to the following lemma.

Lemma 1 *If the process $D(t)$ is ergodic, then the following positive limits exist a.s.*

$$\pi_{i,k} = \lim_{T\to\infty} \frac{\nu_{i,k}(T)}{T} > 0, \qquad (i,k) \in I$$

and satisfy the following system of linear equations

$$v_i^{(-)} - v_k^{(+)} = \sum_{(n,m)\in I_-\times I_+} (\delta(n,i)\mu_i^{(-)} + \delta(m,k)\mu_k^{(+)})\pi_{n,m}, \qquad (i,k) \in I \tag{3}$$

In the ergodic case the correspondence between boundary movement and random walks is completely described by the following theorem.

Theorem 2 *Two following two conditions are equivalent:*
1) The process $D(t)$ is ergodic; *2) $v_L^{(-)} > V$ and $v_K^{(+)} < V$.*

All other cases of boundary movement corresponds to non-ergodic random walks. To understand the corresponding random walk dynamics introduce a new family of processes.

Induced process Let $|J_-| + |J_+|$ families of random variables be given

$$\left\{\theta_{s,i}^{(-)},\ s \in R_+\right\}, \quad (i \in J_-), \qquad \left\{\theta_{s,k}^{(+)},\ s \in R_+\right\}, \quad (k \in J_+). \tag{4}$$

We assume that for any $i \in I_-$ the random variables $\left\{\theta_{s,i}^{(-)},\ s \in R_+\right\}$ are i.i.d., similarly for $\left\{\theta_{s,k}^{(+)},\ s \in R_+\right\}$, and all families (4) are independent of each other.

Define some auxiliary random process $\xi^\Pi(t) = \left(\xi_{i,k}^\Pi(t),\ (i,k) \in \Pi\right)$ with state space $R_+^{|\Pi|}$ and left continuous trajectories, here $\Pi = J_- \times J_+ = \{(i,k) : ...\} \subset I_- \times I_+$:

1) if $\xi_{i,k}^\Pi(t) > 0$ for any $(i,k) \in \Pi$, then

$$\frac{d}{dt}\,\xi_{i,k}^\Pi(t) = v_k^{(+)} - v_i^{(-)} < 0\ , \qquad \forall (i,k) \in \Pi, \tag{5}$$

2) if at some time moment s_0 the coordinate (i_0,k_0) becomes zero, that is $\xi_{i_0,k_0}^\Pi(s_0) = 0$, then the coordinates have jumps as follows:

$$\xi_{n,m}^\Pi(s_0+0) - \xi_{n,m}^\Pi(s_0) = \delta(n,i_0)\theta_{s_0,i_0}^{(-)} + \delta(m,k_0)\theta_{s_0,k_0}^{(+)}, \qquad \forall (n,m) \in \Pi \tag{6}$$

It is clear that $\xi^{\Pi}(t)$ is a Markov process. In $R^{|\Pi|}$ define the linear subspace $\mathcal{D}(R^{|\Pi|})$ of dimension $|J_-| + |J_+| - 1$, by the following system of equations

$$z_{i,k} + z_{n,m} = z_{i,m} + z_{n,k}, \qquad i \neq n, \quad k \neq m.$$

In this system only $(|J_-| - 1)(|J_+| - 1)$ equations are linearly independent. In fact, fix some pair $(i_0, k_0) \in \Pi$. As

$$z_{n,m} = z_{i_0,m} + z_{n,k_0} - z_{i_0,k_0},$$

then any variable can be expressed with $|J_-| + |J_+| - 1$ variables z_{i_0,k_0}, $z_{i_0,m}$ and z_{n,k_0}, $n \neq i_0$, $m \neq k_0$.

Note that if $\xi^{\Pi}(0) \in \mathcal{D}(R^{|\Pi|})$, then for any $t > 0$ $\xi^{\Pi}(t) \in \mathcal{D}(R^{|\Pi|})$.

Relation with the process $D(t)$. Let $\Pi = I_- \times I_+$ and assume that $\theta^{(-)}_{s,i}$ have the same distributions as $u^{(-)}_{j,i}$, and $\theta^{(+)}_{s,k}$ - as $u^{(+)}_{j,k}$. Then it is easy to see that Markov processes $D(t) = (d_{i,k}(t),\ (i,k) \in I_- \times I_+)$ and $\xi^{I_- \times I_+}(t)$ have the same transition kernels.

Let $\Pi = J_- \times J_+ \subsetneq I_- \times I_+$. Consider the restriction $D\Big|_{\Pi}(t) = (d_{i,k}(t),\ (i,k) \in \Pi)$ of the process $D(t) = (d_{i,k}(t),\ (i,k) \in I_- \times I_+)$ on Π. Then this process does not coincide with $\xi^{\Pi}(t)$, starting with $\xi^{\Pi}(0) = D\Big|_{\Pi}(0)$, but even will not be a Markov process. In fact $D\Big|_{\Pi}(t)$ has jumps at time moments when one of the coordinates $(i,k) \in I_- \times I_+$ becomes zero. And $\xi^{\Pi}(t)$ jumps only when becomes zero one of the coordinates from Π. However, if the initial point $D(0)$ is such that each $d_{i,k}(0)$, $(i,k) \in I_- \times I_+ \backslash \Pi$ is sufficiently large, then during some time the processes $D\Big|_{\Pi}(t)$ and $\xi^{\Pi}(t)$ coincide. Thus one can say that $\xi^{\Pi}(t)$ is the "projection" of $D(t)$ far away from the origin. This is quite similar to the notion of the induced process in [1].

Let $\Lambda \subseteq I = I_- \times I_+$. The face of R^N_+ associated with Λ is defined as

$$\mathcal{B}(\Lambda) = \{x \in R^N_+ :\ x_{i,k} > 0,\ (i,k) \in \Lambda,\ x_{i,k} = 0,\ (i,k) \in \overline{\Lambda}\} \subseteq R^N_+$$

If $\Lambda = \emptyset$, then $\mathcal{B}(\Lambda) = \{0\}$. For shortness, instead of $\mathcal{B}(\Lambda)$ we will write Λ.

Consider the faces Λ such that $\overline{\Lambda} = J_- \times J_+$where $J_- \subseteq I_-$и $J_+ \subseteq I_+$. The process $\xi^{\overline{\Lambda}}(t)$ will be called an *induced process*, associated with Λ. Further on we shall use the notation $D_{\Lambda}(t) = (d^{\Lambda}_{i,k}(t), (i,k) \in \overline{\Lambda})$ instead of $\xi^{\overline{\Lambda}}(t)$. The state space of this process is $\mathcal{D}^{\overline{\Lambda}} = \mathcal{D}(R^{|\overline{\Lambda}|})$, where $|\overline{\Lambda}| = |J_-| \times |J_+|$.

Face Λ is called ergodic if the induced process $D_{\Lambda}(t)$ is ergodic.

Denote

$$\nu^{\Lambda}_{i,k}(T) = \#\{t :\ d^{\Lambda}_{i,k}(t) = 0,\ t \in [0,T]\}, \qquad (i,k) \in \overline{\Lambda}$$

Lemma 2 *If the process $D_{\Lambda}(t)$ is ergodic then the following a.e. limits exist and are positive for all pairs $(i,k) \in \overline{\Lambda}$*

$$\pi^{\Lambda}_{i,k} = \lim_{T \to \infty} \frac{\nu^{\Lambda}_{i,k}(T)}{T} > 0 \tag{7}$$

They satisfy the following system of linear equations

$$v^{(-)}_i - v^{(+)}_k = \sum_{(n,m) \in \overline{\Lambda}} (\delta(n,i)\mu^{(-)}_i + \delta(m,k)\mu^{(+)}_k)\pi^{\Lambda}_{n,m},\ (i,k) \in \overline{\Lambda} \tag{8}$$

Let $\overline{\Lambda} = J_- \times J_+ = \{i_l, ..., i_1\} \times \{k_1, ..., k_m\}$, where $i_l > ... > i_1$ and $k_1 < ... < k_m$, and let Λ be an ergodic face. Put $V^{\overline{\Lambda}} = V(J_-, J_+)$. Then

1) $v^{(-)}_{i_l} > V^{\overline{\Lambda}}$ *and* $v^{(+)}_{k_m} < V^{\overline{\Lambda}}$
2) The boundary velocity for the induced process equals (with the a.e. limit)

$$\lim_{t\to\infty} \frac{\beta^{\Lambda}(t)}{t} = V^{\overline{\Lambda}}$$

Note that $V^{\overline{\Lambda}} = V$ for $\Lambda = \emptyset$.

Induced vectors For any ergodic face Λ ($\overline{\Lambda} = J_- \times J_+$) we define the *induced vector* $v^{\Lambda} \in R^N$ with the coordinates equal to

$$v^{\Lambda}_{i,k} = -v^{(-)}_i + v^{(+)}_k + 1(i \in J_-)\mu^{(-)}_i \pi^{(\Lambda,-)}_i + 1(k \in J_+)\mu^{(+)}_k \pi^{(\Lambda,+)}_k$$

where we introduce the following notation

$$\pi^{(\Lambda,-)}_i = \sum_{k\in J_+} \pi^{\Lambda}_{i,k}, \quad i \in J_-; \qquad \pi^{(\Lambda,+)}_k = \sum_{i\in J_-} \pi^{\Lambda}_{i,k}, \quad k \in J_+ .$$

By (8) we have $v^{\Lambda}_{i,k} = 0$ for $(i,k) \in \overline{\Lambda}$, that is the induced vector belongs to the face Λ.

The following lemma explains the meaning of the induced vector.

Lemma 3 *1) The induced vector for the ergodic face* Λ *belongs to* $\mathcal{D} \cap \Lambda$ *and its coordinates are given by*

$$\begin{aligned}
v^{\Lambda}_{i,k} &= -v^{(-)}_i + V^{\overline{\Lambda}}, \qquad (i,k) \in \Lambda, \quad i \notin J_-, \quad k \in J_+ \\
v^{\Lambda}_{i,k} &= v^{(+)}_k - V^{\overline{\Lambda}}, \qquad (i,k) \in \Lambda, \quad i \in J_-, \quad k \notin J_+ \\
v^{\Lambda}_{i,k} &= -v^{(-)}_i + v^{(+)}_k, \qquad (i,k) \in \Lambda, \quad i \notin J_-, \quad k \notin J_+ \\
v^{\Lambda}_{i,k} &= 0, \qquad (i,k) \in \overline{\Lambda}
\end{aligned}$$

2) Let Λ *be ergodic and* $D_y(t)$ *be the Markov process* $D(t)$ *with initial point* y*, that is* $D(0) = y$*. Then for any* $y \in \mathcal{B}(\Lambda)$ *u* $t \geq 0$*, so that* $y + v^{\Lambda} t \in \mathcal{B}(\Lambda)$*, we have*

$$\frac{D_{yN}(tN)}{N} \to y + v^{\Lambda} t$$

a.e. as $N \to \infty$*.*

It follows from condition (2) that for each ergodic face Λ coordinates of the corresponding induced vector $v^{\Lambda}_{i,k} \neq 0$ for all $(i,k) \in \Lambda$.

Non-ergodic faces Let Λ be the face which is not ergodic (non-ergodic face). Ergodic face Λ_1: $\Lambda_1 \supset \Lambda$ will be called outgoing for Λ, if $v^{\Lambda_1}_{i,k} > 0$ for $(i,k) \in \Lambda_1 \setminus \Lambda$.

Let $\mathcal{E}(\Lambda)$ be the set of outgoing faces for the non-ergodic face Λ.

Lemma 4 *The set* $\mathcal{E}(\Lambda)$ *contains the minimal element* Λ_1 *in the sense that for any* $\Lambda_2 \in \mathcal{E}(\Lambda)$ *we have* $\Lambda_2 \supseteq \Lambda_1$.

Dynamical system For any ergodic face Λ we defined the induced vector v^{Λ}, and for any non-ergodic face Λ we defined the vector v^{Λ_1}, where Λ_1 is the minimal element of $\mathcal{E}(\Lambda)$. Thus, we defined the vector field in $\mathcal{D} \cap R_+^N$. Let $T_t x$ be the dynamical system corresponding to this vector field.

We call the ergodic face $\Lambda = \mathcal{L}$ final, if either $\mathcal{L} = \emptyset$ or all coordinates of the induced vector $v^{\mathcal{L}}$ are positive. The central statement is that the dynamical system hits the final face, stays on it forever and goes along it to infinity.

The following theorem, together with theorem 2, is parallel to Theorem 1 and, in all 3 cases of Theorem 1, they exhibit the properties of the corresponding random walks in the orthant.

Theorem 3

1. *Assume*
$$v_K^{(+)} > V$$
Then the process $D(t)$ is transient and there exists a unique ergodic final face $\mathcal{L}_1$, such that $v_{i,k}^{\mathcal{L}_1} > 0$ for $(i,k) \in \mathcal{L}_1$. This face is
$$\mathcal{L}_1(L, K_1) \;=\; \{(i,k) :\; i = 1, ..., L,\; k = K_1 + 1, ..., K\}$$

2. *Assume*
$$v_L^{(-)} < V$$
Then the process $D(t)$ is transient and there exists a unique ergodic final face $\mathcal{L}_2$, such that $v_{i,k}^{\mathcal{L}_2} > 0$ for $(i,k) \in \mathcal{L}_2$. This face is
$$\mathcal{L}_2(L_1, K) \;=\; \{(i,k) :\; i = L_1 + 1, ..., L,\; k = 1, ..., K\}$$

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