75. On the Equation Describing the Random Motion of Mutually Reflecting Molecules

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Introduction. In this paper we construct a model for the random motion of M molecules mutually reflecting in $\boldsymbol{R}^d$ and investigate its limiting behavior as the size R of the molecules tends to 0. We assume that the k-th molecule consists of n_k (≥ 1) atoms. The atoms move randomly in the way as described below (see (0.3)) under the following restrictions (0.1) and (0.2).

(0.1) Any two atoms in different molecules reflect each other when the distance between them equals a given constant ρ (>0).

(0.2) The distance between any two atoms in the same molecule does not exceed a given constant R (>0).

Let $\Lambda=\{1,\cdots,N\}$, $N=\sum_{k=1}^{M} n_k$ and $\Lambda_k=\{\sum_{i=1}^{k-1} n_i+1, \sum_{i=1}^{k-1} n_i+2, \cdots, \sum_{i=1}^{k} n_i\}$, $k=1,\cdots,M$, where the convention $\sum_{i=1}^{0}=0$ is used. Λ_k describes the set of indexes of atoms in the k-th molecule. For each $i\in\Lambda$, we put $m(i)=k$ if $i\in\Lambda_k$. Denote by $X_i(t)$ the position of the i-th atom at time t and put $R_i(t)=\max_{j:m(j)=m(i)}|X_i(t)-X_j(t)|$, $\rho_i(t)=\min_{j:m(j)\neq m(i)}|X_i(t)-X_j(t)|$. We assume that the random motion of the atoms is described by the stochastic differential equation (SDE)

$$dX_i(t)=dB_i(t)+dL_i(t), \quad i=1,2,\cdots,N, \tag{0.3}$$

where $B_i(t)$, $1\leq i\leq N$, are independent d-dimensional Brownian motions and each $L_i(t)$ is a process of bounded variation which can vary only when either $\rho_i(t)=\rho$ or $R_i(t)=R$ and represents effects of (0.1) and (0.2) so that $\rho_i(t)\geq\rho$, $R_i(t)\leq R$, $t\geq 0$, $1\leq i\leq N$. It is assumed that $\rho_i(t)\geq\rho$, $R_i(t)\leq R$, $t\geq 0$, $1\leq i\leq N$. Similar random motions were considered in [3] and [4]; however, in [3] the restriction (0.2) was not considered and in [4] $n_k=1$ for all k.

To solve (0.3) we consider the following problem. For given $\boldsymbol{w}=(w_1, w_2,\cdots,w_N)\in C([0,\infty)\to\boldsymbol{R}^{Nd})$ satisfying

$$\begin{aligned}|w_i(0)-w_j(0)|&\leq R \quad \text{for all} \quad i,j \quad \text{with} \quad m(i)=m(j),\\ &\geq\rho \quad \text{for all} \quad i,j \quad \text{with} \quad m(i)\neq m(j),\end{aligned}$$

we want to find $\xi_i^R(t)$ satisfying the equation

$$\xi_i^R(t)=w_i(t)+\sum_{\substack{j=1\\(\neq i)}}^{N}\int_0^t(\xi_i^R(s)-\xi_j^R(s))dl_{ij}^R(s) \quad i=1,2,\cdots,N, \tag{0.4}$$

under the following conditions (i) and (ii):

(i) $\xi^R=(\xi_1^R,\xi_2^R,\cdots,\xi_N^R)\in C([0,\infty)\to\boldsymbol{R}^{Nd})$ with

$$|\xi_i^R(t)-\xi_j^R(t)|\leq R \quad \text{for all} \quad i, j \quad \text{with} \quad m(i)=m(j),$$
$$\geq \rho \quad \text{for all} \quad i, j \quad \text{with} \quad m(i)\neq m(j), \quad t\geq 0,$$

(ii) l_{ij}^R is a continuous function which is nonincreasing or nondecreasing according as $m(i)=m(j)$ or $m(i)\neq m(j)$; moreover $l_{ij}^R=l_{ji}^R$, $l_{ij}^R(0)=0$ and

$$l_{ij}^R(t)=\begin{cases}\int_0^t \mathbf{1}_{\{|\xi_i^R(s)-\xi_j^R(s)|=R\}}(s)dl_{ij}^R(s), & \text{if } m(i)=m(j),\\ \int_0^t \mathbf{1}_{\{|\xi_i^R(s)-\xi_j^R(s)|=\rho\}}(s)dl_{ij}^R(s), & \text{if } m(i)\neq m(j),\end{cases}$$

where $\mathbf{1}_A$ denotes the indicator function of a set A.

If we have a unique solution $\xi_i^R(t)=\xi_i^R(t, w_1, \cdots, w_N)$ of (0.4) for each given $\boldsymbol{w}=(w_1, \cdots, w_N)$, we obtain a stochastic process $\boldsymbol{X}(t)=(X_1(t), \cdots, X_N(t))$ where $X_i(t)=\xi_i^R(t, W_1, \cdots, W_N)$, W_i being defined by $W_i(t)=X_i(0)+B_i(t)$, $1\leq i\leq N$. Then the process $\boldsymbol{X}(t)$ satisfies the SDE (0.3) and is what we call the *random motion of M molecules mutually reflecting* in $\boldsymbol{R}^d$. We show that the equation (0.4) can be solved uniquely employing the idea in [4]. That is, we prove that the domain

$$\mathcal{D}_R=\{x=(x_1, x_2, \cdots, x_N)\in \boldsymbol{R}^{Nd}: |x_i-x_j|<R \text{ for } \forall i, j \text{ with } m(i)=m(j)$$
$$\text{and } >\rho \text{ for } \forall i, j \text{ with } m(i)\neq m(j)\}$$

satisfies Conditions (A) and (B) in § 1 which assure the existence of the unique solution of the Skorohod problem $(w; \mathcal{D}_R)$ and then we derive the equation (0.4) from the Skorohod equation for $(w; \mathcal{D}_R)$. We also show that the unique solution ξ^R of (0.4) converges to some limit ξ^0 as $R\downarrow 0$. In the limit motion ξ^0 all the atoms belonging to the i-th molecule perform the same motion which is denoted by η_i^0. Then $\eta^0=(\eta_1^0, \cdots, \eta_M^0)$ may be regarded as describing the random motion of mutually reflecting M hard balls of diameter ρ with different masses.

In § 1 we first state the results on Skorohod problem for general domains following [1] and then, the solvability of the equation (0.4). The convergence of ξ^R is stated in § 2 and the characterization of the limiting function is given in § 3. Details of the proofs and some related results will appear elsewhere.

§ 1. Skorohod problem and the solvability of (0.4). Let D be a domain in $\boldsymbol{R}^n$ and we call $\boldsymbol{n}\in\boldsymbol{R}^n$ an inward unit normal vector at $x\in\partial D$ if $|\boldsymbol{n}|=1$ and $B(x-r\boldsymbol{n}, r)\cap D=\emptyset$ for some $r>0$, where $B(y,r)=\{z\in\boldsymbol{R}^n: |y-z|<r\}$. We denote the set of inward unit normal vectors at $x\in\partial D$ by $\mathcal{N}_x=\mathcal{N}_x(D)$ and set $\mathcal{N}_{x,r}\equiv\mathcal{N}_{x,r}(D)=\{\boldsymbol{n}: |\boldsymbol{n}|=1, B(x-r\boldsymbol{n}, r)\cap D=\emptyset\}$, $r>0$. We introduce the following two conditions on D.

Condition (A). *There exists a positive constant* r_D *such that*

$$\mathcal{N}_x=\mathcal{N}_{x,r_D}\neq\emptyset \qquad \text{for all } x\in\partial D.$$

Condition (B). *There exist constants* $\delta>0$ *and* $\beta\in[1,\infty)$ *with the following property; for any* $x\in\partial D$ *there exists a unit vector* $\boldsymbol{e}_x$ *such that*

$$\langle \boldsymbol{e}_x, \boldsymbol{n}\rangle\geq 1/\beta \qquad \text{for all } \boldsymbol{n}\in\bigcup_{y\in B(x,\delta)\cap\partial D}\mathcal{N}_y,$$

where $\langle\cdot,\cdot\rangle$ *is the usual inner product in* $\boldsymbol{R}^n$.

Following Lions and Sznitman [1] and Saisho [2] we consider the following Skorohod problem.

Skorohod problem $(w; D)$. Given $w \in C([0,\infty)\to \boldsymbol{R}^n)$ with $w(0) \in \bar{D}$, find a pair (ξ, l) of functions satisfying the equation

$$\xi(t)=w(t)+\int_0^t \boldsymbol{n}(s)dl(s) \tag{1.1}$$

under the conditions:

(i) $\xi \in C([0,\infty)\to \bar{D})$,

(ii) l is a continuous nondecreasing function with $l(0)=0$ and $l(t)=\int_0^t \mathbf{1}_{\partial D}(\xi(s))dl(s)$,

(iii) $\boldsymbol{n}(s) \in \mathcal{N}_{\xi(s)}$ if $\xi(s) \in \partial D$.

When we refer to the *Skorohod problem* $(w; D)$ or the *Skorohod equation* (1.1) *for* $(w; D)$, we always consider (1.1) under these conditions (i), (ii) and (iii). The following theorem is known.

Theorem 1.1 ([2]). *If D satisfies Conditions* (A) *and* (B), *for any $w \in C([0,\infty)\to \boldsymbol{R}^n)$ with $w(0) \in \bar{D}$, the Skorohod problem $(w; D)$ can be solved uniquely.*

We now proceed to the special case where $D=\mathcal{D}_R$.

Proposition 1.1. *If $0<R<\rho/4$, then the domain $\mathcal{D}_R$ satisfies Conditions* (A) *and* (B) *with $r_{\mathcal{D}}\equiv r_{\mathcal{D}_R}=\{\sqrt{N}(18M-15)\rho\}^{-1}R^2$ and*

$$\mathcal{N}_x(\mathcal{D}_R)=\{\boldsymbol{n}: |\boldsymbol{n}|=1,\ \boldsymbol{n}=\sum_{(i,j)\in \boldsymbol{J}_x} c_{ij}\boldsymbol{n}_{ij}(x),\ c_{ij}\geq 0\}, \quad x \in \partial\mathcal{D}_R,$$

where $\boldsymbol{J}_x=\{(i,j): 1\leq i<j\leq N, |x_i-x_j|=R \text{ or } =\rho\}$ and

$$\boldsymbol{n}_{ij}(x)=\begin{cases}\Big(0,\cdots,0,\underset{(i\text{-th})}{\dfrac{x_j-x_i}{\sqrt{2}R}},0,\cdots,0,\underset{(j\text{-th})}{\dfrac{x_i-x_j}{\sqrt{2}R}},0,\cdots,0\Big), & \text{if } m(i)=m(j),\\ \Big(0,\cdots,0,\underset{(i\text{-th})}{\dfrac{x_i-x_j}{\sqrt{2}\rho}},0,\cdots,0,\underset{(j\text{-th})}{\dfrac{x_j-x_i}{\sqrt{2}\rho}},0,\cdots,0\Big), & \text{if } m(i)\neq m(j),\end{cases} \quad x\in\partial\mathcal{D}_R.$$

By virtue of Proposition 1.1 we can make use of Theorem 1.1 to obtain the existence of a unique solution of the Skorohod problem $(w; \mathcal{D}_R)$, Moreover, we can prove that the equation (0.4) is equivalent to the Skorohod equation for $(w; \mathcal{D}_R)$ and consequently obtain the following theorem.

Theorem 1.2. *For each $0<R<\rho/4$, the equation* (0.4) *has a unique solution.*

We now put

$$\mathcal{D}_\infty=\{x=(x_1,x_2,\cdots,x_N)\in \boldsymbol{R}^{Nd}: |x_i-x_j|>\rho,\ m(i)\neq m(j)\},$$

$$\mathcal{O}=\{x=(x_1,x_2,\cdots,x_M)\in \boldsymbol{R}^{Md}: |x_i-x_j|>\rho\}.$$

We remark here the following for the later use.

Remark 1.1. (1)([3]) $\mathcal{D}_\infty$ satisfies Conditions (A) and (B) with $r_\infty\equiv r_{\mathcal{D}_\infty}=\rho\{8(N-1)^{3/2}\}^{-1}$ and

$$\mathcal{N}_x(\mathcal{D}_\infty)=\{\boldsymbol{n}: |\boldsymbol{n}|=1,\ \boldsymbol{n}=\sum_{(i,j)\in \boldsymbol{J}_x^\infty} c_{ij}\boldsymbol{n}_{ij}(x),\ c_{ij}\geq 0\}, \quad x\in\partial\mathcal{D}_\infty,$$

where $\boldsymbol{J}_x^\infty=\{(i,j): 1\leq i<j\leq N, |x_i-x_j|=\rho,\ m(i)\neq m(j)\}$.

(2)([3], [4]) $\mathcal{O}$ satisfies Conditions (A) and (B) with $r_{\mathcal{O}}=\rho\{8(M-1)^{3/2}\}^{-1}$ and

$$\mathcal{N}_x(\mathcal{O})=\{\boldsymbol{n}: |\boldsymbol{n}|=1,\ \boldsymbol{n}=\sum_{(k,h)\in J_x^{\mathcal{O}}} c_{kh}\boldsymbol{m}_{kh}(x),\ c_{kh}\geq 0\},\quad x\in\partial\mathcal{O},$$

where $J_x^{\mathcal{O}}=\{(k,h): 1\leq k<h\leq M, |x_k-x_h|=\rho\}$ and

$$\boldsymbol{m}_{kh}(x)=\Big(0,\cdots,0,\underset{(k\text{-th})}{\frac{x_k-x_h}{\sqrt{2}\,\rho}},0,\cdots,0,\underset{(h\text{-th})}{\frac{x_h-x_k}{\sqrt{2}\,\rho}},0,\cdots,0\Big).$$

§ 2. Convergence of ξ^R as R tends to 0. Let $\xi^R(t)=w(t)+\int_0^t \boldsymbol{n}(s)dl^R(s)$ be the Skorohod equation for $(w;\mathcal{D}_R)$. Then by Proposition 1.1, we can write

(2.1) $$\xi^R(t)=w(t)+\psi^R(t)+\varphi^R(t).$$

where

$$\psi^R(t)=\int_0^t \sum_{\substack{1\leq i<j\leq N\\ m(i)=m(j)}} c_{ij}(s)\boldsymbol{n}_{ij}(s)dl^R(s),\quad \varphi^R(t)=\int_0^t \sum_{\substack{1\leq i<j\leq N\\ m(i)\neq m(j)}} c_{ij}(s)\boldsymbol{n}_{ij}(s)dl^R(s).$$

Remark 2.1. (2.1) is the Skorohod equation for $(w+\psi^R;\mathcal{D}_\infty)$, that is, we can write (2.1) in the form:

$$\xi^R(t)=w(t)+\psi^R(t)+\int_0^t \boldsymbol{m}(s)d\tilde{l}^R(s),\quad \boldsymbol{m}(s)\in\mathcal{N}_{\xi^R(s)}(\mathcal{D}_\infty)\quad\text{if } \xi^R(s)\in\partial\mathcal{D}_\infty.$$

For any $x\in\boldsymbol{R}^{Md}$ we define $\bar{x}=(\bar{x}_1,\bar{x}_2,\cdots,\bar{x}_N)\in\boldsymbol{R}^{Nd}$ by $\bar{x}_i=x_k$ if $m(i)=k$, and for $f:[0,\infty)\to\boldsymbol{R}^{Md}$ we define $\bar{f}:[0,\infty)\to\boldsymbol{R}^{Nd}$ by $\bar{f}(t)=\overline{f(t)}$, $t\in[0,\infty)$. Next, for $x\in\boldsymbol{R}^{Nd}$ we define $G(x)\in\boldsymbol{R}^{Md}$ by $(G(x))_k=\sum_{i\in A_k} x_i/n_k$, $k=1,2,\cdots,M$, and denote $\eta^R=G(\xi^R)$, $\Phi^R=G(\varphi^R)$, $\tilde{w}=G(w)$ and $\overline{w}=\bar{\tilde{w}}$. Clearly, η^R describes the motion of the center of gravity of each molecule. Furthermore, we use the following notation; for a continuous function u defined on $[0,\infty)$, we set

$$\triangle_{s,t}(u)=\sup\{|u(t_1)-u(t_2)|: s\leq t_1<t_2\leq t\},$$
$$\|u\|_t=\sup\{|u(s)|: 0\leq s\leq t\},$$
$$|u|_t=\text{the total variation of } u \text{ on } [0,t],$$
$$|u|_t^s=|u|_t-|u|_s,\quad 0\leq s\leq t.$$

Then we note that (2.1) implies $\eta^R(t)=\tilde{w}(t)+\Phi^R(t)$ and $\overline{\eta^R}(t)=\overline{w}(t)+\overline{\Phi^R}(t)$. Setting $\varphi^R(t)=\int_0^t \boldsymbol{m}(s)d\tilde{l}^R(s)$, we can prove the following proposition.

Proposition 2.1. *Let $T>0$ be any finite time. Then for sufficiently small $R>0$, there exist positive constants K_1 and K_2 such that*

$$|\varphi^R|_t^s\leq K_1\triangle_{s,t}(\overline{w})+K_2R\Big(1+\frac{R}{r_\infty}\Big),\quad 0\leq s<t\leq T,$$

where K_1, K_2 depend only on ρ, T, $\|\overline{w}\|_T$ and the modulus of uniform continuity of $\overline{w}$.

For the proof we employ an argument similar to that in the proof of Proposition 3.1 of [2].

Remark 2.2. For sufficiently small $R>0$, Proposition 2.1 implies that $|\varphi^R|_t$, $|\overline{\Phi^R}|_t$ are uniformly bounded in R for any finite $t>0$.

Lemma 2.1. *Suppose that ξ^R and $\xi^{R'}$ solve the Skorohod equations $\xi^R(t)=w(t)+\psi^R(t)+\varphi^R(t)$ and $\xi^{R'}(t)=w(t)+\psi^{R'}(t)+\varphi^{R'}(t)$, for $(w+\psi^R;\mathcal{D}_\infty)$, $(w+\psi^{R'};\mathcal{D}_\infty)$, respectively. Then, we have*

(2.2) $$|\overline{\eta^R}(t)-\overline{\eta^{R'}}(t)|^2 \leq \frac{2}{r_\infty}\int_0^t |\overline{\eta^R}(s)-\overline{\eta^{R'}}(s)|^2(d|\varphi^R|_s+d|\varphi^{R'}|_s)$$
$$+2(R+R')\left\{\sqrt{N}+\frac{1}{r_\infty}(R+R')N\right\}(|\varphi^R|_t+|\varphi^{R'}|_t), \quad t\geq 0.$$

Using Proposition 2.1, Lemma 2.1 and Gronwall's lemma we get the following theorem.

Theorem 2.1. *$\overline{\eta^R}$ converges uniformly on each finite t-interval as $R \downarrow 0$.*

The following theorem is immediate from Theorem 2.1 and the fact $|\xi_i^R(t)-\overline{\eta_i^R}(t)|\leq R$, $1\leq i\leq N$.

Theorem 2.2. *ξ^R coverges uniformly on each finite t-interval as $R \downarrow 0$.*

§ 3. Characterization of the limiting function. By Theorem 2.1, we have $\overline{\eta^R}\to\xi^0$ and $\overline{\Phi^R}\to\overline{\Phi^0}$ uniformly in $t\in[0,T]$ as $R\downarrow 0$ for some limiting functions ξ^0 and $\overline{\Phi^0}$, respectively for any finite $T>0$. Here we remark that $\xi_i^0=\xi_j^0$ for all i, j with $m(i)=m(j)$ and if we define $\eta^0=(\eta_1^0,\eta_2^0,\cdots,\eta_M^0)\in \boldsymbol{R}^{Md}$ by $\eta_k^0=\xi_i^0$ for i with $m(i)=k$, $k=1,2,\cdots,M$, we have $\overline{\eta^0}=\xi^0$. Using the method of [2: Theorem 4.1] we can show

(1°) $\quad d\overline{\Phi^0}(s)=\tilde{\boldsymbol{n}}(s)d|\overline{\Phi^0}|_s,\quad \tilde{\boldsymbol{n}}(s)\in \mathcal{N}_{\overline{\eta^0}(s)}(\mathcal{D}_\infty)\quad$ if $\xi^0(s)\in\partial\mathcal{D}_\infty$,

(2°) $\quad \int_0^t \tilde{\boldsymbol{n}}(s)d|\overline{\Phi^0}|_s=\overline{\Phi^0}(t),$

from which the following theorem is obtained.

Theorem 3.1. *ξ^0 solves the Skorohod problem $(\overline{w};\mathcal{D}_\infty)$, that is, $\xi^0(t)=\overline{w}(t)+\overline{\Phi^0}(t)$ is a Skorohod equation.*

Remark 3.1. We can also prove that $\tilde{\boldsymbol{n}}(s)$ in (1°) is written in the form:

$$\tilde{n}_i(s)=\sum_{\substack{j=1\\(\neq i)}}^N \tilde{c}_{ij}(s)(\xi_i^0(s)-\xi_j^0(s)),\quad \tilde{c}_{ij}(s)\geq 0,\ i=1,2,\cdots,N.$$

Thus, we can write

$$\xi_i^0(t)=\overline{w}_i(t)+\int_0^t\sum_{\substack{j=1\\(\neq i)}}^N \tilde{c}_{ij}(s)(\xi_i^0(s)-\xi_j^0(s))d|\overline{\Phi^0}|_s,\quad i=1,2,\cdots,N.$$

Setting $\overline{l_{ij}^0}(t)=\int_0^t \tilde{c}_{ij}(s)d|\overline{\Phi^0}|_s$ and then $l_{kh}^0(t)=\overline{l_{ij}^0}(t)$ for $k=m(i)$, $h=m(j)$, we easily have the following theorem.

Theorem 3.2. *$\{\eta^0(t)\}$ is a unique solution of*

(3.1) $$\eta_k^0(t)=\tilde{w}_k(t)+\sum_{\substack{h=1\\(\neq k)}}^M n_h\int_0^t(\eta_k^0(s)-\eta_h^0(s))dl_{kh}^0(s),\quad k=1,2,\cdots,M,$$

with the conditions that

(1) *$\eta^0=(\eta_1^0,\eta_2^0,\cdots,\eta_M^0)\in C([0,\infty)\to\boldsymbol{R}^{Md})$ and $|\eta_k^0(t)-\eta_h^0(t)|\geq\rho$ if $k\neq h$,*

(2) *l_{kh}^0 is a continuous nondecreasing function with $l_{kh}^0=l_{hk}^0$, $l_{kh}^0(0)=0$, and*

$$l_{kh}^0(t)=\int_0^t \mathbf{1}_{\{|\eta_k^0(s)-\eta_h^0(s)|=\rho\}}(s)dl_{kh}^0(s).$$

In particular, if $n_1=n_2=\cdots=n_M$, $\{\eta^0(t)\}$ solves the Skorohod problem $(\tilde{w};\mathcal{O})$.

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