Interacting particle systems with sticky boundary

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Introduction

Let $\Omega \subset \mathbb{R}^d$, $d \geq 1$, be a bounded domain with smooth boundary Γ. Denote by λ the Lebesgue measure on Ω, by σ the surface measure on Γ and let $\alpha \in C^1(\overline{\Omega})$, $\alpha > 0$.

Then the solution of the following SDE describes a distorted Brownian motion in Ω with (immediate) reflection at Γ:

$$d\tilde{\mathbf{X}}_t = d\tilde{B}_t + \frac{1}{2}\frac{\nabla\alpha}{\alpha}(\tilde{\mathbf{X}}_t)dt - \frac{1}{2}\alpha(\tilde{\mathbf{X}}_t)n(\tilde{\mathbf{X}}_t)\, dl_t^{\tilde{\mathbf{X}}},\qquad \tilde{\mathbf{X}}_0 = x \in \overline{\Omega},$$

where $(\tilde{B}_t)_{t\geq 0}$ is an $\mathbb{R}^d$-valued standard Brownian motion, $(l_t^{\tilde{\mathbf{X}}})_{t\geq 0}$ is the boundary local time and n the outward normal.

Let $\beta \in C(\overline{\Omega})$, $\beta > 0$, and define the additive functional $(A_t)_{t\geq 0}$ by $A_t := t + \int_0^t \beta(\tilde{\mathbf{X}}_s)dl_s^{\tilde{\mathbf{X}}}$, $t \geq 0$. Using the inverse $(\tau(t))_{t\geq 0}$ of $(A_t)_{t\geq 0}$ it is possible to define the time changed process $(\mathbf{X}_t)_{t\geq 0}$, $\mathbf{X}_t := \tilde{\mathbf{X}}_{\tau(t)}$, which is a solution of the SDE

$$d\mathbf{X}_t = \mathbb{1}_\Omega(\mathbf{X}_t)\big(dB_t + \frac{1}{2}\frac{\nabla\alpha}{\alpha}(\mathbf{X}_t)dt\big) - \frac{1}{2}\,\mathbb{1}_\Gamma(\mathbf{X}_t)\frac{\alpha}{\beta}(\mathbf{X}_t)n(\mathbf{X}_t)\, dt,\qquad \mathbf{X}_0 = x \in \overline{\Omega},$$

where $(B_t)_{t\geq 0}$ is an $\mathbb{R}^d$-valued standard Brownian motion. This follows by $\int_0^t \mathbb{1}_\Gamma(\tilde{\mathbf{X}}_s)\, ds = 0$ a.s. for every $t \geq 0$.
$(\mathbf{X}_t)_{t\geq 0}$ is called a sticky reflected distorted Brownian motion or distorted Brownian motion with delayed reflection, since the new time scale slows the process down if it reaches Γ. Moreover, the process spends indeed time on Γ in the sense

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t \mathbb{1}_\Gamma(\mathbf{X}_s)\, ds = c > 0 \quad \text{a.s. for some fixed constant } c.$$

The Dirichlet form associated to the distorted Brownian motion with immediate reflection is given by the closure $(\tilde{\mathcal{E}}, D(\tilde{\mathcal{E}}))$ of

$$\tilde{\mathcal{E}}(f,g) = \frac{1}{2}\int_\Omega (\nabla f, \nabla g)\, \alpha d\lambda, \quad f,g \in C^1(\overline{\Omega}), \quad \text{on } L^2(\overline{\Omega};\alpha\lambda).$$

The local time $(l_t^{\tilde{\mathbf{X}}})_{t\geq 0}$ is in Revuz correspondence with the surface measure σ and therefore, the Revuz measure of $(A_t)_{t\geq 0}$ is given by $\alpha\lambda + \beta\sigma$. As a consequence, the Dirichlet form $(\mathcal{E}, D(\mathcal{E}))$ associated to the sticky reflected distorted Brownian motion is given by the closure of $(\tilde{\mathcal{E}}, C^1(\overline{\Omega}))$ on $L^2(\overline{\Omega};\alpha\lambda + \beta\sigma)$.

In the following, we present step by step the Dirichlet form construction of a system of N interacting sticky reflected distorted Brownian motions on $\overline{\Omega}$ for $N \in \mathbb{N}$ under mild assumptions on the boundary Γ, the interaction and the densities α and β. Since the process spends indeed time on Γ, we provide additionally an optional diffusion along Γ. This interacting particle system provides a model for the dynamics of molecules in a chromatography tube.

Dirichlet form for a single particle

Let $\Omega \subset \mathbb{R}^d$, $d \geq 1$, be a bounded domain with boundary Γ.

Condition C1

Γ is Lipschitz continuous. Moreover, let $\alpha \in L^1(\Omega;\lambda)$, $\alpha > 0$ λ-a.e., and $\beta \in L^1(\Gamma;\sigma)$, $\beta > 0$ σ-a.e.

Set $\varrho = \mathbb{1}_\Omega\alpha + \mathbb{1}_\Gamma\beta$ and $\mu := \alpha\lambda + \beta\sigma = \varrho(\lambda + \sigma)$.

Define $(\mathcal{E}, C^1(\overline{\Omega}))$ on $L^2(\overline{\Omega};\mu)$ by

$$\mathcal{E}(f,g) := \frac{1}{2}\int_\Omega (\nabla f, \nabla g)\, \alpha d\lambda + \frac{\delta}{2}\int_\Gamma (\nabla_\Gamma f, \nabla_\Gamma g)\, \beta d\sigma = \frac{1}{2}\int_{\overline{\Omega}} \big(\mathbb{1}_\Omega\, (\nabla f, \nabla g) + \delta\, \mathbb{1}_\Gamma\, (\nabla_\Gamma f, \nabla_\Gamma g)\big)\, d\mu$$

for $f,g \in C^1(\overline{\Omega})$, where $\delta \in \{0,1\}$, $P(x) := E - n(x)n(x)^t$ and $\nabla_\Gamma f(x) := P(x)\nabla f(x)$ for $f \in C^1(\overline{\Omega})$, $x \in \Gamma$. Let

$$R_\alpha(\Omega) := \{x \in \Omega |\ \int_{\{y\in\Omega|\ |x-y|<\epsilon\}} \alpha^{-1}d\lambda < \infty \ \text{ for some } \epsilon > 0\}$$

and analogously $R_\beta(\Gamma)$.

Condition C2 (Hamza condition)

$\alpha = 0$ λ-a.e. on $\Omega\backslash R_\alpha(\Omega)$ and if $\delta = 1$ $\beta = 0$ σ-a.e. on $\Gamma\backslash R_\beta(\Gamma)$.

Proposition 1

Assume that C1 and C2 are fulfilled. Then $(\mathcal{E}, C^1(\overline{\Omega}))$ is densely defined and closable on $L^2(\overline{\Omega};\mu)$. Its closure $(\mathcal{E}, D(\mathcal{E}))$ is a conservative, strongly local, regular, symmetric Dirichlet form.

Generator for a single particle

Condition C3

Γ is Lipschitz continuous and $\alpha, \beta \in C(\overline{\Omega})$, $\alpha > 0$ λ-a.e. on Ω, $\beta > 0$ σ-a.e. on Γ such that $\sqrt{\alpha} \in H^{1,2}(\Omega)$. Additionally, Γ is C^2-smooth and $\sqrt{\beta} \in H^{1,2}(\Gamma)$ if $\delta = 1$.

C3 implies C1 and C2. Note that C3 yields $\frac{|\nabla\alpha|}{\alpha} \in L^2(\Omega;\alpha\lambda)$ and if $\delta = 1$ also $\frac{|\nabla_\Gamma\beta|}{\beta} \in L^2(\Gamma;\beta\sigma)$.

Proposition 2

Assume that C3 is fulfilled and denote by $(L, D(L))$ the generator of $(\mathcal{E}, D(\mathcal{E}))$. Then $C^2(\overline{\Omega}) \subset D(L)$ and

$$Lf = \frac{1}{2}\,\mathbb{1}_\Omega\big(\Delta f + (\frac{\nabla\alpha}{\alpha}, \nabla f)\big) - \frac{1}{2}\,\mathbb{1}_\Gamma\frac{\alpha}{\beta}(n, \nabla f) + \delta\,\frac{1}{2}\,\mathbb{1}_\Gamma\big(\Delta_\Gamma f + (\frac{\nabla_\Gamma\beta}{\beta}, \nabla_\Gamma f)\big)$$

for $f \in C^2(\overline{\Omega})$.

For $\delta = 0$ this is connected to the *Wentzell boundary condition*

$$\alpha(n, \nabla f) = \beta\,\big(\Delta f + (\frac{\nabla\alpha}{\alpha}, \nabla f)\big) \text{ on } \Gamma.$$

Dynamics of a single particle

Theorem 1

Assume that C3 is fulfilled. Then there exists a conservative diffusion process (i.e. a strong Markov process with continuous sample paths and infinite life time)

$$\mathbf{M} = \big(\mathbf{\Omega}, \mathcal{F}, (\mathcal{F}_t)_{t\geq 0}, (\mathbf{X}_t)_{t\geq 0}, (\Theta_t)_{t\geq 0}, (\mathbf{P}_x)_{x\in\overline{\Omega}}\big)$$

with state space $\overline{\Omega}$ which is properly associated with $(\mathcal{E}, D(\mathcal{E}))$ on $L^2(\overline{\Omega};\mu)$ and $\mathbf{M}$ is a solution to the SDE

$$\begin{aligned} d\mathbf{X}_t &= \mathbb{1}_\Omega(\mathbf{X}_t)\big(dB_t + \frac{1}{2}\frac{\nabla\alpha}{\alpha}(\mathbf{X}_t)dt\big) - \frac{1}{2}\,\mathbb{1}_\Gamma(\mathbf{X}_t)\frac{\alpha}{\beta}(\mathbf{X}_t)n(\mathbf{X}_t)\, dt \\ &\quad + \delta\,\mathbb{1}_\Gamma(\mathbf{X}_t)\big(dB_t^\Gamma + \frac{1}{2}\frac{\nabla_\Gamma\beta}{\beta}(\mathbf{X}_t)dt\big), \qquad (\#) \\ dB_t^\Gamma &= P(\mathbf{X}_t)\circ dB_t = P(\mathbf{X}_t)dB_t - \frac{1}{2}\kappa(\mathbf{X}_t)\, n(\mathbf{X}_t)\, dt, \\ \mathbf{X}_0 &= x \in \overline{\Omega}, \end{aligned}$$

for quasi every $x \in \overline{\Omega}$, where $\kappa = \mathrm{div}_\Gamma n$ $(-\kappa\, n = (P\nabla)^t P)$.

If we require additional assumptions on α and β, the statement of the Theorem 1 can be strengthened:

Condition C4

C3 is fulfilled. Furthermore, Γ is C^2-smooth, $\mathrm{cap}(\{\varrho = 0\}) = 0$ and there exists $p \geq 2$, $p > d$, such that

$$\frac{|\nabla\alpha|}{\alpha} \in L^p_{\mathrm{loc}}(\overline{\Omega} \cap \{\varrho > 0\};\alpha\lambda)$$

and if $\delta = 1$

$$\frac{|\nabla_\Gamma\beta|}{\beta} \in L^p_{\mathrm{loc}}(\Gamma \cap \{\varrho > 0\};\beta\sigma).$$

Theorem 2

Suppose that C4 is fulfilled. Then the statement of Theorem 1 holds accordingly, but $\mathbf{M}$ is a strong Feller process with state space $\overline{\Omega} \cap \{\varrho > 0\}$ and Dirichlet form $(\mathcal{E}, D(\mathcal{E}))$ on $L^2(\overline{\Omega} \cap \{\varrho > 0\};\mu)$. Moreover, it solves the SDE (#) for every $x \in \overline{\Omega} \cap \{\varrho > 0\}$.

The proof of Theorem 2 is based on the general construction scheme presented in [1] using regularity results for elliptic PDEs with Wentzell boundary conditions.

Product form of N pre-Dirichlet forms

Let α_i and β_i, $i = 1,\ldots,N$, fulfill C1 and C2. Denote by $(\mathcal{E}^i, C^1(\overline{\Omega}))$ the according forms. Define $(\otimes_{i=1}^N \mathcal{E}^i, C^1(\Lambda))$, $\Lambda := \overline{\Omega}^N$, by

$$\otimes_{i=1}^N \mathcal{E}^i(f,g) := \sum_{i=1}^N \int_{\overline{\Omega}^{N-1}} \mathcal{E}^i(f,g) \prod_{j\neq i}(\alpha_j\lambda_j + \beta_j\sigma_j)$$

for $f,g \in C^1(\Lambda)$. This bilinear form is closable on $L^2(\Lambda;\mu^N)$, where $\mu^N := \prod_{i=1}^N(\alpha_i\lambda_i + \beta_i\sigma_i)$. Its closure is a regular Dirichlet form and yields N independent sticky reflected distorted Brownian motions. Next we introduce an interaction.

General Dirichlet form for N particles

$(\otimes_{i=1}^N \mathcal{E}^i, C^1(\Lambda))$ has the representation

$$\frac{1}{2}\int_\Lambda \sum_{i=1}^N \big(\mathbb{1}_{\Lambda^{i,\Omega}}\,(\nabla_i f, \nabla_i g) + \delta\,\mathbb{1}_{\Lambda^{i,\Gamma}}\,(\nabla_{i,\Gamma} f, \nabla_{i,\Gamma} g)\big)\, d\mu^N,$$

where $\Lambda^{i,\Omega} := \{x = (x^1,\ldots,x^N) \in \Lambda |\ x^i \in \Omega\}$, $\Lambda^{i,\Gamma}$ similary, and ∇_i denotes the gradient w.r.t. the i-th component in $\Lambda = \overline{\Omega}^N$ for $i = 1,\ldots,N$.

Let $\phi \in C(\Lambda)$ and $\phi > 0$ μ^N-a.e. Define

$$\mathcal{G}(f,g) := \frac{1}{2}\int_\Lambda \sum_{i=1}^N \big(\mathbb{1}_{\Lambda^{i,\Omega}}(\nabla_i f, \nabla_i g) + \delta\mathbb{1}_{\Lambda^{i,\Gamma}}(\nabla_{i,\Gamma} f, \nabla_{i,\Gamma} g)\big)\ \phi d\mu^N$$

for $f,g \in C^1(\Lambda)$.

Proposition 3

Assume that α_i and β_i, $i = 1,\ldots,N$ fulfill C1 and C2. Let $\phi \in C(\Lambda)$ and $\phi > 0$ μ-a.e. Then $(\mathcal{G}, C^1(\Lambda))$ is densely defined and closable on $L^2(\Lambda;\phi\,\mu)$. Its closure $(\mathcal{G}, D(\mathcal{G}))$ is a conservative, strongly local, regular, symmetric Dirichlet form.

Note that in contrast to the case of an immediate reflection the construction for $N > 1$ can not be reduced to the case $N = 1$.

Dynamics of the interacting particle system

Condition C5

$\phi \in C^1(\Lambda)$, $\phi > 0$ μ-a.e., such that $\frac{|\nabla\phi|}{\phi} \in L^2(\Lambda;\phi\,\mu)$.

Set $\varrho_i := \mathbb{1}_\Omega\alpha_i + \mathbb{1}_\Gamma\beta_i$, $i = 1,\ldots,N$.

Theorem 3

Assume that α_i and β_i, $i = 1,\ldots,N$, fulfill C3 and ϕ fulfills C5. Then there exists a conservative diffusion process $\mathbf{M}^N$ with state space Λ which is properly associated with $(\mathcal{G}, D(\mathcal{G}))$. $\mathbf{M}^N$ is for quasi every $x \in \Lambda$ a solution to the SDE

$$\begin{aligned} d\mathbf{X}_t^i &= \mathbb{1}_\Omega(\mathbf{X}_t^i)\Big(dB_t^i + \frac{1}{2}\big(\frac{\nabla_i\alpha_i}{\alpha_i}(\mathbf{X}_t^i) + \frac{\nabla_i\phi}{\phi}(\mathbf{X}_t)\big)dt\Big) - \frac{1}{2}\mathbb{1}_\Gamma(\mathbf{X}_t^i)\frac{\alpha_i}{\beta_i}(\mathbf{X}_t^i)n(\mathbf{X}_t^i)dt \\ &\quad + \delta\,\mathbb{1}_\Gamma(\mathbf{X}_t^i)\Big(dB_t^{\Gamma,i} + \frac{1}{2}\big(\frac{\nabla_{\Gamma,i}\beta_i}{\beta_i}(\mathbf{X}_t^i) + \frac{\nabla_{\Gamma,i}\phi}{\phi}(\mathbf{X}_t)\big)dt\Big), \\ dB_t^{\Gamma,i} &= P(\mathbf{X}_t^i)\circ dB_t^i = P(\mathbf{X}_t^i)dB_t^i - \frac{1}{2}\kappa(\mathbf{X}_t^i)\, n(\mathbf{X}_t^i)\, dt, \quad i = 1,\ldots,N \\ \mathbf{X}_0 &= x \in \Lambda. \end{aligned}$$

Suppose additionally that α_i and β_i, $i = 1,\ldots,N$, fulfill C4 and that ϕ is strictly positive. Then it exists a solution for every $x \in \Lambda_1 := \Lambda \setminus \{x = (x^1,\ldots,x^N) \in \Lambda |\ \prod_{i=1}^N \varrho_i(x^i) = 0\}$.

Note that the above SDE has in general no strong solution by [2].

Application

In [3] a similar system of interacting particles with sticky boundary was constructed in view of a model for the dynamics in a chromatography tube, but the interaction is in particular assumed to be bounded and Lipschitz continuous. Our construction even allows singular interactions. E.g. it is possible to consider ϕ given by

$$\phi(x^1,\ldots,x^N) := \exp\big(-\sum_{\substack{1\leq i,j\leq N\\ i\neq j}} V(|x^i - x^j|)\big),$$

where $V(r) := r^{-12} - r^{-6}$, $r > 0$, denotes the Lennard-Jones potential.

References and Acknowledgment

[1] B. Baur, M. Grothaus and P. Stilgenbauer. Construction of $\mathcal{L}^p$-strong Feller Processes via Dirichlet Forms and Applications to Elliptic Diffusions. *Potential Anal.*, 38(4):1233-1258, 2013.

[2] H. -J. Engelbert and G. Peskir. Stochastic differential equations for sticky Brownian motion. In *Research report No. 5, 2012, Probability and Statistics Group*, pages 28 pp., School of Mathematics, The University of Manchester, 2012.

[3] C. Graham. The martingale problem with sticky reflection conditions, and a system of particles interacting at the boundary. *Ann. Inst. Henri Poincaré Probab. Stat.*, 24(1):45-72, 1988.

[4] R. Voßhall. Interacting particle system with sticky boundary. *arXiv:1508.02519*, 2015.

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