A mechanical model of Brownian motion including low energy light particles

Song Liang(梁松)
(Waseda University(早稲田大学), Japan)

2019/7/11–15
Jilin, China
(15th Workshop on Markov Processes and Related Topics)

Motivation

Explanation of Brownian motion

A rough explanation : A grain of pollen immersed into a glass of water
$\longrightarrow$ A result of the repeated collisions of the massive particle with the numerous lighter but faster light particles (the water molecules)
$\longrightarrow$ IF the states(positions and velocities) of the light particles (for the same time and between different times) are INDEPENDENT, then OK by CLT (Central Limit Theorem)

Explanation of Brownian motion

A rough explanation : A grain of pollen immersed into a glass of water
$\longrightarrow$ A result of the repeated collisions of the massive particle with the numerous lighter but faster light particles (the water molecules)
$\longrightarrow$ IF the states(positions and velocities) of the light particles (for the same time and between different times) are INDEPENDENT, then OK by CLT (Central Limit Theorem)

BUT : the interaction also affects the motion of the light particles (especially in a potential interaction model)
$\longrightarrow$ INDEPENDENT assumption NOT satisfied!

Motivation

Explanation of Brownian motion

A rough explanation : A grain of pollen immersed into a glass of water
$\longrightarrow$ A result of the repeated collisions of the massive particle with the numerous lighter but faster light particles (the water molecules)
$\longrightarrow$ IF the states(positions and velocities) of the light particles (for the same time and between different times) are INDEPENDENT, then OK by CLT (Central Limit Theorem)

BUT : the interaction also affects the motion of the light particles (especially in a potential interaction model)
$\longrightarrow$ INDEPENDENT assumption NOT satisfied!

Our aim : Consider a system that evolves according to a classical Newtonian dynamics (which is consistent with the mentioned dependence on the past), and study the behavior of the massive particle when the mass of the light particles converges to 0.

Our dynamical model

- $\mathbf{R}^d$ $(d > 1)$
- massive particle: one, with mass 1,
- light particles: ideal gas (definition given later), mass m $(m \to 0)$,
- initial condition $(X(0), V(0)) \in \mathbf{R}^d \times \mathbf{R}^d$ and $\tilde{\omega} \in \mathit{Conf}(\mathbf{R}^d \times \mathbf{R}^d)$,

  the set of all non-empty closed subsets of $\mathbf{R}^d \times \mathbf{R}^d$ with no cluster point,

  here $(x, v) \in \tilde{\omega}$ means that there exists a light particle with initial position x and initial velocity v,
- as long as the initial condition $(X(0), V(0)) \in \mathbf{R}^d \times \mathbf{R}^d$ and $\tilde{\omega} \in \mathit{Conf}(\mathbf{R}^d \times \mathbf{R}^d)$ is given, the system is totally deterministic and Newtonian, with its Hamiltonian given by

$$\frac{1}{2}|V|^2 + \sum_{(x,v)\in\tilde{\omega}} \frac{m}{2}|v|^2 + \sum_{(x,v)\in\tilde{\omega}} U(X - x)$$

Here $U \in C_0^\infty(\mathbf{R}^d)$ is the potential function.

ODEs of the system

- Massive particle: one, mass 1, with its state (position and velocity) at time t written as $(X(t), V(t))$
- light particles: mass m, the state of a light particle with initial condition (x, v) at time t is written as $(x(t, x, v), v(t, x, v))$

$$
\begin{cases}
\frac{d}{dt} X^{(m)}(t, \widetilde{\omega}) = V^{(m)}(t, \widetilde{\omega}), \\
\frac{d}{dt} V^{(m)}(t, \widetilde{\omega}) = - \sum_{(x,v) \in \widetilde{\omega}} \nabla U(X^{(m)}(t, \widetilde{\omega}) - x^{(m)}(t, x, v, \widetilde{\omega})), \\
(X^{(m)}(0, \widetilde{\omega}), V^{(m)}(0, \widetilde{\omega})) = (X_0, V_0), \\
\\
\frac{d}{dt} x^{(m)}(t, x, v, \widetilde{\omega}) = v^{(m)}(t, x, v, \widetilde{\omega}), \\
m \frac{d}{dt} v^{(m)}(t, x, v, \widetilde{\omega}) = \nabla U(X^{(m)}(t, \widetilde{\omega}) - x^{(m)}(t, x, v, \widetilde{\omega})), \\
(x^{(m)}(0, x, v, \widetilde{\omega}), v^{(m)}(0, x, v, \widetilde{\omega})) = (x, v), \qquad (x, v) \in \widetilde{\omega}.
\end{cases}
$$

initial distribution of the environmental light particles

$\widetilde{P_m}(d\widetilde{\omega}) \in \wp(Conf(\mathbf{R}^d \times \mathbf{R}^d))$: Poisson point process with intensity

$$\widetilde{\lambda_m}(dx, dv) = m^{\frac{d-1}{2}} \rho\Big(\frac{m}{2}|v|^2, x - X_0\Big) dxdv,$$

Definition

$\widetilde{P_m}(d\widetilde{\omega})$ is the PPP with intensity $\widetilde{\lambda_m}$ iff

- for any $A \in \mathcal{B}(\mathbf{R}^d \times \mathbf{R}^d)$, $\sharp(\widetilde{\omega} \cap A)$ (the number of light particles with their initial conditions $(x, v) \in A$) is a random variable with Poisson distribution $Po(\widetilde{\lambda_m}(A))$,
- for any $A, B \in \mathcal{B}(\mathbf{R}^d \times \mathbf{R}^d)$ compact, disjoint, $\sharp(\widetilde{\omega} \cap A)$ and $\sharp(\widetilde{\omega} \cap B)$ are independent

- So both the density and the velocities of the light particles are of order $m^{-\frac{1}{2}}$

Assumptions

Assumption w.r.t. U: $U \in C_0^\infty(\mathbf{R}^d)$, spherical-symmetric, repulsive, precisely,

(U1) $\exists R_U > 0$, $\exists h : [0,\infty) \to [0,\infty)$, *s.t.*,

- $U(x) = h(|x|)$, $\forall x \in \mathbf{R}^d$,
- $U(x) = 0$ if $|x| \geq R_U$,
- $h'(a) < 0$, $\forall a \in (0, R_U)$,
- $h''(0) < 0$.

Assumptions w.r.t. ρ:

(A1) $\exists \overline{E} > 0$ *s.t.* $\rho(u,z) = 0$ as long as $u + U(z) < \overline{E}$.
$\longrightarrow$ The initial energies of the light particles are bounded below

(A2) $\rho(u,-z) = \rho(u,z)$, $\forall z \in \mathbf{R}^d$, $u \in [0,\infty)$. $\exists \rho_0 : [0,\infty) \to [0,\infty)$, $\exists R_1 > 0$ *s.t.* $\rho(u,z) = \rho_0(u)$ if $|z| \geq R_1$, $u \in [0,\infty)$.
$\longrightarrow$ The initial distribution of the light particles is symmetric, and except the very first duration, the distribution of the incoming light particles does not dependent on the massive particle

(A3) $\int_{\mathbf{R}^d} (1+|v|^3) \sup_{z\in\mathbf{R}^d} \rho(\frac{1}{2}|v|^2, z) dv < \infty$. $\longrightarrow$ A integrability of ρ

Literature

- Holley (1971): $d = 1$, interaction=collision
- Dürr-Goldstein-Lebowitz (1980–1983), Calderoni-Dürr-Kusuoka (1989): $d \geq 1$, interaction=collision
- simulation, e.g., Kim-Karniadakis (2015)
- Kusuoka-Liang (2010), Liang (2014): plural massive particles, interaction=potential interaction,
  initial energies of all light particles are "high enough"
  ($\Leftrightarrow$ initial velocities of all light particles are "fast enough")
  $\Longrightarrow$ the interactions are not strong enough to "stop the light particles", so all light particles "pass through" their effective interaction ranges, hence the effective interaction time durations of all light particles are short enough

Ray representation (Idea 1)

gives us the approximate time that the corresponding light particle enters its effective interaction range!

- $E = \{(y,v) \in \mathbf{R}^d \times (\mathbf{R}^d \setminus \{0\});\ y \cdot v = 0\}$,
- $E_v = \{y \in \mathbf{R}^d; y \cdot v = 0\}, \qquad v \in \mathbf{R}^d \setminus \{0\}$,
- $\Psi : \mathbf{R} \times E \to \mathbf{R}^d \times (\mathbf{R}^d \setminus \{0\}), (s,(y,v)) \mapsto \Psi(s,(y,v)) = (y - sv, v)$,
- $\nu(dy,dv) \in \wp(E)$: $\nu(dy,dv) = |v|\widetilde{\nu}(dy;v)dv$, here $\widetilde{\nu}(dy;v)$ is the Lebesgue measure on E_v,
- $\Omega = Conf(\mathbf{R} \times E)$,
- $P_m(d\omega) = P_{\lambda_m}(d\omega)$: Poisson point process on $Conf(\mathbf{R} \times E)$ with intensity $\lambda_m(dr,dy,dv) \in \wp(\Omega)$:

$$\lambda_m(dr,dy,dv) = m^{-1}\rho\Big(\frac{1}{2}|v|^2, y - m^{-1/2}rv - X_0\Big)dr\nu(dy,dv),$$

Freezing-approximation (Idea 2) (Main idea of Kusuoka-L.(2010), L.(2014))

When considering the evolution of each one light particle,

since the velocity of a light particles is of order $m^{-\frac{1}{2}}$ and the velocity of the massive particle is of order 1,

if the initial energy of a light particle is large enough, *i,.e,*,

if $|v| \geq m^{-\frac{1}{2}}(2C_0 + 1)$, here $C_0 := \sqrt{2R_U \|\nabla U\|_\infty}$, then

- the effective interaction time duration is short enough
- so the massive particle almost does not move during this period
- so we can approximate the evolution of the light particle by the one that the massive particle is frozen ($\leftarrow$ our freezing-approximation)

Freezing-approximation (Idea 2) (Main idea of Kusuoka-L.(2010), L.(2014))

When considering the evolution of each one light particle,

since the velocity of a light particles is of order $m^{-\frac{1}{2}}$ and the velocity of the massive particle is of order 1,

if the initial energy of a light particle is large enough, *i,.e,*,

if $|v| \geq m^{-\frac{1}{2}}(2C_0 + 1)$, here $C_0 := \sqrt{2R_U \|\nabla U\|_\infty}$, then

- the effective interaction time duration is short enough
- so the massive particle almost does not move during this period
- so we can approximate the evolution of the light particle by the one that the massive particle is frozen ($\leftarrow$ our freezing-approximation)

Notice:

- If the initial energy of the light particle is NOT high enough, then the sojourn time of even the freezing-approximation might be ∞!
  (Example : if the light particle comes exactly towards the massive particle, and with its initial energy = the maximum of the potential function)

Formulation of the limiting process(I)

- (our "freezing approximation") for any $(x,v) \in \mathbf{R}^{2d}$ and $X \in \mathbf{R}^d$,

$$\begin{cases} \frac{d}{dt}\varphi^0(t,x,v;X) = \varphi^1(t,x,v;X) \\ \frac{d}{dt}\varphi^1(t,x,v;X) = -\nabla U(\varphi^0(t,x,v;X) - X) \\ (\varphi^0(0,x,v;X), \varphi^1(0,x,v;X)) = (x,v). \end{cases}$$

(the same as the ODEs with respect to the light particles with the massive particle frozen and with $m = 1$)

- (scattering) $\psi(t,x,v;X) := \lim_{s\to\infty} \varphi^0(t+s, x-sv, v; X)$, $(x,v) \in E$.
- (first order approximation error of our freezing-approximation) for any $(x,v) \in E, X, V \in \mathbf{R}^d, a \in \mathbf{R}$, let $z(t;x,v,X,V,a)$ be the solution of

$$\begin{cases} \frac{d^2}{dt^2} z(t) = -\nabla^2 U(\psi^0(t,x,v,X) - X)\Big(z(t) - (t+a)V\Big), \\ \lim_{t\to-\infty} z(t) = \lim_{t\to-\infty} \frac{d}{dt} z(t) = 0. \end{cases}$$

Remark: $z(t;x,v,X,V,a)$ is linear with respect to V.

$$x(m^{1/2}t + s, \Psi(s,x,m^{-1/2}v)) \approx \psi^0(t,x,v;X(s-c_m)) \\ + m^{1/2} z(t,x,v;X(s-c_m), V(s-c_m), m^{-1/2}c_m)$$

Formulation of the limiting process(II)

- The generator of our limiting process:

$$L = \frac{1}{2}\sum_{k,l=1}^{d} a_{kl}\frac{\partial^2}{\partial V_k \partial V_l} + \sum_{k,l=1}^{d} b_{kl} V_l \frac{\partial}{\partial V_k} + \sum_{k=1}^{d} V_k \frac{\partial}{\partial X_k}.$$

$$\begin{aligned} a_{kl} &= \int_E \Big(\int_{-\infty}^{\infty} \nabla_k U(\psi^{\mathbf{0}}(t,x,v;X)-X)dt\Big) \\ &\qquad \times \Big(\int_{-\infty}^{\infty} \nabla_l U(\psi^{\mathbf{0}}(t,x,v;X)-X)dt\Big)\rho_{\mathbf{0}}(\frac{1}{2}|v|^{\mathbf{2}})\nu(dx,dv), \\ \sum_{l=\mathbf{1}}^{d} b_{kl}V_l^{\ell} &= -\int_E \Big(\int_{-\infty}^{\infty} \nabla^{\mathbf{2}} U(\psi^{\mathbf{0}}(t,x,v,X)-X) \\ &\qquad \times z(t,x,v,X,V,-t)dt\Big)\rho_{\mathbf{0}}(\frac{1}{2}|v|^{\mathbf{2}})\nu(dx,dv). \end{aligned}$$

Remark

- a and b correspond to the 0-order and the 1-order of our freezing-approximation,
- (since there is only one massive particle now), a and b do not depend on X indeed.
- coincide with the model with collision interaction

Main result

Our metric on $C([0,\infty);\mathbf{R}^{2d})$: for any $w_1, w_2 \in \mathbf{R}^{2d}$,
$dist(w_1,w_2) := \sum_{k=1}^{\infty} 2^{-k}\Big(1 \wedge \max_{t\in[0,k]} |w_1(t) - w_2(t)|\Big)$.

Theorem

Assume (A1)–(A3) and (U1). Also, assume that

$$d > \sqrt{\frac{\|h''\|_\infty}{-h''(0)}} + \sqrt{\frac{\|h''\|_\infty}{-h''(0)} + 1}. \quad (1)$$

Then when $m \to 0$, the distribution of $\{(X^{(m)}(t), V^{(m)}(t)); t \geq 0\}$ under $\widetilde{P}_m$ converges to the diffusion process with generator L in $(C([0,\infty);\mathbf{R}^{2d}), dist)$.

Remark When $-h''(0) = \|h''\|_\infty$, then (1) is satisfied as long as $d \geq 3$.

(In a previous paper of L. (2018), we needed $d > 2(1 + \|h''\|_\infty)(-h''(0))^{-\frac{1}{2}} + 1$, which implies $d \geq 6$ at least).

Sketch of the proof (I)

Suffice to prove for $t \in [0, T \wedge \sigma_n]$. Here $\sigma_n := \inf\{t > 0; |V_t| \geq n\}$.

1. Ray representation,
2. Freezing-approximation: approximate $x(s, \Psi(r, x, m^{-\frac{1}{2}}v))$ by $\varphi^0(m^{-\frac{1}{2}}s, \Psi(m^{-\frac{1}{2}}r, x, v; X))$ or $\psi^0(m^{-\frac{1}{2}}(s-r), x, v; X)$, where
   - $X = X(0)$ when proving that the force during the very first short duration (definition given later) is negligible,
   - $X = X(\tilde{r})$ when estimating the effective interaction duration of the light particle and when a measurable approximation is necessary,
   - $X = X(s)$ when proving the convergence in the last step.
3. Decompose $V(t)$ as

   $$V(t) = \text{a martingale term} + \text{a smooth term} + \text{a negligible term},$$

   and prove the tightness of each term (in the Skorohod space).
4. Prove the convergence of each term, so the limiting process is a solution of the martingale problem L, (that is, the distribution of $\{f(X(t \wedge \sigma_n), V(t \wedge \sigma_n)) - f(X_0, V_0) - \int_0^{t \wedge \sigma_n} Lf(X(s), V(s))ds;\ t \in [0, T]\}$ is a martingale for any $f \in C_0^\infty(\mathbf{R}^d \times \mathbf{R}^d)$). So OK by the martingale problem theory.

Sketch of the proof (II)

5. Remove the singular light particles:
   $|x - \pi_v^\perp X(\tilde{r})| \geq m^\alpha$ and $|v| \geq m^{\frac{\gamma}{2}}$. $(\tilde{r} \approx r - m^{\frac{1}{2}}\tau)$
   - $\alpha > \frac{1}{2(d-1)}$ and $\gamma > \frac{1}{d+1} \longrightarrow$ The total affect from those light particles that do not satisfy these conditions is small enough
   - $\alpha(3\sqrt{C_1/\varepsilon_1} - d + 1) < \frac{1}{2}$ and $\sqrt{C_1/\varepsilon_1}(2\alpha + \gamma) < 1 \longrightarrow$ All light particles satisfying these conditions leave the effective interaction range within a time duration short enough, hence the approximation errors of our freezing approximations are small enough
6. Estimation of the effective interaction time duration:

$$t_1(v, y) := \exists C_2 + 1_{\{|v|<2C_0\}}\varepsilon_1^{-1/2}\log^+\left(\exists C_3|v|^{-1}y^{-1}\right).$$

both the freezing approximation and the light particle could be in the effective interaction range only during $[-\tau, t_1(v, |x - \pi_v^\perp X(\cdot)|)]$.

- Proof for the freezing approximation: use two invariants: the total energy and $(\varphi^0 - X, \varphi^1)^2 - |\varphi^0 - X|^2|\varphi^1|^2$
- Proof for the light particle: use the result for freezing approximation and the error estimate

Remark: Our error estimate has an exponential order w.r.t. the effective interaction time duration, so the log-order here is essential!

Further Possible Generalizations

1. $\overline{E} = 0$ (*i,.e,*, no minimum constraint of the initial energies of the light particles):
   $\longrightarrow$ The effective interaction time duration is not of log order any more
   $\longrightarrow$ Some more accurate estimate necessary. In progress now.
2. A model with the potential diverges to infinity at 0 (for example, the Weeks-Chandler-Andersen potential or the Lennard-Jones potential):
   $\longrightarrow$ $\nabla^2 U$ is not bounded, so the error estimate of the positions is not enough to apply the estimate of the difference between forces
   $\longrightarrow$ Expected that the method for Problem 1 is applicable

Reference

1. S. Kusuoka and S. Liang, *A classical mechanical model of Brownian motion with plural particles,* Rev. Math. Phys. 22, no. 7, 733–838 (2010)
2. A mechanical model of Brownian motion for one massive particle including slow light particles, J. Stat. Phys. 170, no. 2, 286–350 (2018)
3. A mechanical model of Brownian motion for one massive particle including slow light particles in dimension $d \geq 3$, Preprint

4. P. Calderoni, D. Dürr, and S. Kusuoka, *A mechanical model of Brownian motion in half-space,* J. Statist. Phys. 55, no. 3-4, 649–693 (1989)
5. D. Dürr, S. Goldstein, and J. L. Lebowitz, *A mechanical model of Brownian motion,* Comm. Math. Phys. 78, no. 4, 507–530 (1980/81)
6. D. Dürr, S. Goldstein, and J. L. Lebowitz, *A mechanical model for the Brownian motion of a convex body,* Z. Wahrsch. Verw. Gebiete 62, no. 4, 427–448 (1983)
7. D. Dürr, S. Goldstein, and J. L. Lebowitz, *Stochastic processes originating in deterministic microscopic dynamics,* J. Statist. Phys. 30, no. 2, 519–526 (1983)
8. R. Holley, *The motion of a heavy particle in an infinite one dimensional gas of hard spheres,* Z. Wahrscheinlichkeitstheorie und Verw. Gebiete, 17, 181–219 (1971)

Thank you!