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Diffusion and Classical Dynamics

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Brownian motion, which was first observed by Brown in 1827, is a well-known physical phenomenon concerning the dynamics of a small particle immersed into a fluid in equilibrium, *e.g.*, a grain of pollen in a glass of water [15]. It is always an interesting problem in mathematical physics to describe the Brownian motion phenomenology by classical mechanical models.

The first physical explanation of Brownian motion was given by Einstein: the motion is coming about as a result of the repeated collisions of the massive particle with the numerous much smaller but faster fluid atoms. In more mathematical terms the explanation is often presented in the following rough way: since the massive particle is collided by a big number of very light water particles, if we could assume that the interactions from each light particle at each time are independent, then by the central limit theorem for the sum of *i.i.d.* random variables, this will give in a suitable limit the Brownian motion.

However, this assumption of independence can hardly be justified, even in a model where only interactions through collisions are considered, since there exists the possibility of re-collisions. This becomes a more evident and significant drawback when considering the model of interactions caused by potentials. Therefore, the actual motion of the massive particle can not be explained as resulting from a sum of *i.i.d.* random variables, it is not even a Markov process.

So in order to study this phenomenon more precisely, one needs to construct some model which is consistent with the mentioned dependence on the past. In such a model, a massive particle interacts with a gas of infinitely many light particles, with the dynamics fully deterministic and Newtonian, as long as the initial condition is given. The only source of randomness is from the initial configuration of the light particles. The problem we will be concerned with is to describe the motion of the massive particle in the Brownian limit, where the mass m of the light particles goes to 0, while the density and the velocities of them have order $m^{-1/2}$. The scaling is done in such a way that the variance of the momentum transfer stays of order 1. See the introductions of [12] and [13] for a more detailed explanation with respect to the reason of this scaling.

This type of model, called a mechanical model of Brownian motion, was first introduced and studied by Holley [9], for the case where the whole system is in dimension $d = 1$, and the interactions are given by collisions. This model was later extended by, *e.g.*, Dürr-Goldstein-Lebowitz [6], [7], [8], Calderoni-Dürr-Kusuoka [2], to the case of higher dimensional spaces. Szász-Tóth [16] also considered some related problem. We notice that in all these papers, the interactions were just of the collisions type.

We consider such a model where the interactions between the massive particle and the light particles are given by a spherical-symmetric compactly supported smooth potential function U. So we are assuming the following:

U1. $U \in C_0^\infty(\mathbf{R}^d)$, and there exists a constant $R_U > 0$ and a smooth function $h : [0, \infty) \to [0, \infty)$ such that $U(x) = h(|x|)$ for any $x \in \mathbf{R}^d$ and $U(x) = 0$ if $|x| \geq R_U$.

Write the initial condition of our system as (X_0, V_0) and $\tilde{\omega}$: (X_0, V_0) is the initial state (*i.e.*, the position and the velocity) of the massive particle, and $\tilde{\omega} \in Conf(\mathbf{R}^d \times \mathbf{R}^d)$ gives us the initial condition of the light particles – $(x, v) \in \tilde{\omega}$ means that there exists an environmental particle with position x and velocity v at time 0. Here $Conf(*)$ stands for the set of all nonempty closed subsets of $*$ which have no cluster point. The distribution of $\tilde{\omega}$ will be given later. As soon as the initial condition of the system is given, our system is totally deterministic, Newtonian, with the Hamilton given by $\frac{1}{2}|V|^2 + \sum_{(x,v)} \frac{m}{2}|v|^2 + \sum_{(x,v)} U(X-x)$.

For any initial condition $\tilde{\omega}$ and time $t \in [0,\infty)$, let $(X^{(m)}(t,\tilde{\omega}), V^{(m)}(t,\tilde{\omega}))$ denote the state of the massive particle at time t, and for any $(x,v) \in \tilde{\omega}$, let $(x^{(m)}(t,x,v,\tilde{\omega}), v^{(m)}(t,x,v,\tilde{\omega}))$ denote the state at time t of the light particle which had state (x,v) at time 0. So our dynamical system is given by the following infinite system of ordinary differential equations:

$$
\begin{cases}
\dfrac{d}{dt}X^{(m)}(t,\tilde{\omega}) = V^{(m)}(t,\tilde{\omega}), \\
\dfrac{d}{dt}V^{(m)}(t,\tilde{\omega}) = -\displaystyle\int_{\mathbf{R}^d\times\mathbf{R}^d} \nabla U(X^{(m)}(t,\tilde{\omega}) - x^{(m)}(t,x,v,\tilde{\omega}))\mu_{\tilde{\omega}}(dx,dv), \\
(X^{(m)}(0,\tilde{\omega}), V^{(m)}(0,\tilde{\omega})) = (X_0, V_0), \\
\\
\dfrac{d}{dt}x^{(m)}(t,x,v,\tilde{\omega}) = v^{(m)}(t,x,v,\tilde{\omega}), \\
m\dfrac{d}{dt}v^{(m)}(t,x,v,\tilde{\omega}) = -\nabla U(x^{(m)}(t,x,v,\tilde{\omega}) - X^{(m)}(t,\tilde{\omega})), \\
(x^{(m)}(0,x,v,\tilde{\omega}), v^{(m)}(0,x,v,\tilde{\omega})) = (x,v), \qquad (x,v)\in\tilde{\omega}.
\end{cases}
\tag{1}
$$

Here $\mu_{\tilde{\omega}}(\;\cdot\;)$ is the counting measure determined by $\tilde{\omega}$: $\mu_{\tilde{\omega}}(A) = \sharp(\tilde{\omega}\cap A)$ for any $A \in \mathcal{B}(\mathbf{R}^d \times \mathbf{R}^d)$. ($\sharp(\;\cdot\;)$ thus denoting the number of points in the argument).

The only randomness of our model comes from the distribution of the environmental initial condition $\tilde{\omega}$, which is given by the following. Let ρ : $[0,\infty)\times\mathbf{R}^d \to [0,\infty)$ be a measurable function such that $\sup_{z\in\mathbf{R}^d}\rho(u,z) \to 0$ rapidly as $u\to\infty$. Let $\widetilde{\lambda_m}$ be the non-atomic Radon measure on $\mathbf{R}^d\times\mathbf{R}^d$ given by

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

and let $\widetilde{P_m}(d\tilde{\omega})$ be the Poisson point process with the intensity measure $\widetilde{\lambda_m}$. So $\widetilde{P_m}$ is a probability measure on $\widetilde{\Omega} = Conf(\mathbf{R}^d\times\mathbf{R}^d)$. We assume that the distribution of $\tilde{\omega}$ is given by $\widetilde{P_m}$. (See, *e.g.*, [10] for more details with respect to Poisson point processes).

We assume the following assumptions with respect to ρ:

A1. There exists a constant $\overline{v} > 0$ such that $\rho(u, z) = 0$ for any $u < \frac{1}{2}\overline{v}^2$ and $z \in \mathbf{R}^d$.

A2. $\rho(u, -z) = \rho(u, z)$ for any $z \in \mathbf{R}^d$ and $u \in [0, \infty)$. Also, there exist a function $\rho_0 : [0, \infty) \to [0, \infty)$ and a constant $R_1 > 0$ such that $\rho(u, z) = \rho_0(u)$ as long as $|z| \geq R_1$ for any $u \in [0, \infty)$.

A3. $\int_{\mathbf{R}^d} (1 + |v|^3) \rho_{max}(\frac{1}{2}|v|^2) dv < \infty$. Here $\rho_{max}(u) := \sup_{z \in \mathbf{R}^d} \rho(u, z)$, $u \in [0, \infty)$.

Although as explained, the behavior of the massive particle is not Markovian, we notice that one expects that the non-Markovian character of the dynamics disappears when $m \to 0$, heuristically because at least when the initial velocities of light particles are fast enough, the effective interaction durations should be short enough.

As announced, we are going to prove that under certain condition, when $m \to 0$, the distribution of the stochastic process $\{(X^{(m)}(t), V^{(m)}(t)); t \in [0, \infty)\}$ converges weakly to a diffusion, with our metric on $C([0, \infty); \mathbf{R}^{2d})$ given by

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

Let us start our discussion with a technical assumption that all light particles are sufficiently fast. Precisely, we assume for a while that the constant $\overline{v}$ of (A1) satisfies $\overline{v} \geq 2C_0 + 1$, with $C_0 := \sqrt{2R_U \|\nabla U\|_\infty}$. As proved in [12], this assumption ensures that all light particles cross the effective interaction range in a bounded time, and never reenter the valid range. Therefore, when considering the behavior of the light particles, we could use the approximation that the massive particle is frozen. This is the so-called freezing approximation, see φ and ψ defined below.

We prepare several notations in order to formulate our limiting process. First of all, for any $X \in \mathbf{R}^d$ and $(x,v) \in \mathbf{R}^{2d}$, let $\varphi(t,x,v;X) = (\varphi^0(t,x,v;X), \varphi^1(t,x,v;X))$ denote the solution of the following system of ordinary differential equations:

$$\begin{cases} \dfrac{d}{dt}\varphi^0(t,x,v;X) = \varphi^1(t,x,v;X) \\ \dfrac{d}{dt}\varphi^1(t,x,v;X) = -\nabla U(\varphi^0(t,x,v;X) - X) \\ (\varphi^0(0,x,v;X), \varphi^1(0,x,v;X)) = (x,v). \end{cases} \tag{2}$$

We notice that (2) is the same as the second half of (1) with $m = 1$, except that the quantity $X^{(1)}(t)$ of (1) is substituted by X in (2).

Next, let

$$\begin{aligned} E &= \{(x,v) \in \mathbf{R}^d \times (\mathbf{R}^d \setminus \{0\});\ x \cdot v = 0\}, \\ E_v &= \{x \in \mathbf{R}^d; x \cdot v = 0\}, \qquad v \in \mathbf{R}^d \setminus \{0\}, \end{aligned}$$

and let $\nu(dx,dv)$ be the measure on E given by $\nu(dx,dv) = |v|\tilde{\nu}(dx;v)dv$, where $\tilde{\nu}(dx;v)$ is the Lebesgue measure on E_v. We define the ray representation Ψ as follows:

$$\begin{aligned} \Psi : \qquad & \mathbf{R} \times E \to \mathbf{R}^d \times (\mathbf{R}^d \setminus \{0\}), \\ & (s,(x,v)) \mapsto \Psi(s,(x,v)) = (x - sv, v). \end{aligned} \tag{3}$$

In words, we decompose the position of each environmental particle into two parts: one parallel to its velocity and the other orthogonal to its velocity. We remark that in this new space $\mathbf{R} \times E$, v is still the initial velocity of the light particle, while x is not the initial position of it anymore: now x is only the component of its initial position that is perpendicular to the velocity. Also, s gives us approximately the time that this particle enters the effective interaction range.

For any $X \in \mathbf{R}^d$ and $(x,v) \in E$, we have that

$$\psi(t,x,v;X) := (\psi^0(t,x,v;X), \psi^1(t,x,v;X)) := \lim_{s\to\infty} \varphi(t+s, x - sv, v; X) \tag{4}$$

is well-defined. As explained, $\varphi^0(m^{\frac{1}{2}}t, \Psi(m^{-\frac{1}{2}}, x, v); X)$ and $\psi(t - m^{-\frac{1}{2}}r, x, v; X)$ with some proper X are our freezing-approximations of $x(t, \Psi(r, x, m^{-\frac{1}{2}}v))$.

Also, for any $(x, v) \in E$, $X, V \in \mathbf{R}^d$ and $a \in \mathbf{R}$, let $z(t; x, v, X, V, a)$ denote the solution of

$$\begin{cases} \frac{d^2}{dt^2} z(t) = -\nabla^2 U(\psi^0(t, x, v, X) - X)\Big(z(t) - (t + a)V\Big), \\ \lim_{t\to-\infty} z(t) = \lim_{t\to-\infty} \frac{d}{dt} z(t) = 0. \end{cases} \tag{5}$$

$z(t; x, v, X, V, a)$ with proper X, V and a gives us the first order of the approximation error of our freezing-approximation. We notice that $z(t; x, v, X, V, a)$ is a linear function of V.

Our limiting diffusion generator L on function over $\mathbf{R}^{2d}$ is given by the following:

$$L = \frac{1}{2} \sum_{k,l=1}^{d} a_{kl} \frac{\partial^2}{\partial V_k \partial V_l} + \sum_{k,l=1}^{d} b_{kl} V_l \frac{\partial}{\partial V_k} + \sum_{k=1}^{d} V_k \frac{\partial}{\partial X_k}, \tag{6}$$

with

$$\begin{aligned} a_{kl} &= \int_E \Big(\int_{-\infty}^{\infty} \nabla_k U(\psi^0(t, x, v; X) - X) dt \Big) \\ &\qquad \times \Big(\int_{-\infty}^{\infty} \nabla_l U(\psi^0(t, x, v; X) - X) dt \Big) \rho_0(\frac{1}{2}|v|^2) \nu(dx, dv), \end{aligned}$$

and $b_{kl} : \mathbf{R}^d \to R$, $k, l = 1, \cdots, d$, are C^∞-functions determined by the following relation:

$$\begin{aligned} &- \int_E \Big(\int_{-\infty}^{\infty} \nabla^2 U(\psi^0(t, x, v, X) - X) z(t, x, v, X, V, -t) dt \Big) \rho_0(\frac{1}{2}|v|^2) \nu(dx, dv) \\ &= \sum_{l=1}^{d} b_{kl} V_l^{\ell}. \end{aligned}$$

The coefficients a and b correspond to the 0-order and the 1-order approximations, respectively, of our freezing-approximation. We notice that as proved in [13, pages 248–249], since there is only one massive particle in our model, a and b are indeed independent of X, so our limiting process coincides with that for the model with hard core (see [6]). We also remark that the integrals with respect to t in the definitions of a_{kl} and b_{kl} are finite.

Now we are ready to formulate our first result.

Theorem 1 (**[12]**) *Assume (U1), (A2) and (A3). Also, assume (A1) with* $\overline{v} \geq 2C_0 + 1$. *Then when* $m \to 0$, *the distribution of* $\{(X^{(m)}(t), V^{(m)}(t)); t \geq 0\}$ *under* $\widetilde{P_m}$ *converges weakly to the diffusion process with generator* L *in* $(C([0,\infty);\mathbf{R}^{2d}), dist)$.

Remark 2 *To be precise, [12] considered a more general model where there might be more than one massive particles, as a result, (when restrict it to the case where their is only one massive particle as in our present model) the assumption in [12] with respect to* ρ *is actually a special case of our model: [12] assumed that there exists a* $\overline{\rho}$ *such that* $\rho(u,x) = \overline{\rho}(u + U(z - X_0))$ *for any* $(u,z) \in [0,\infty) \times \mathbf{R}^d$, *and that* $\overline{\rho}(s) = 0$ *for any* $s \leq \frac{1}{2}(2C_0+1)^2 + \|U\|_\infty$. *Nevertheless, we can get Theorem 1 by using exactly the same method and estimates of [12].*

[13] also considered this model under the assumption that all light particles are sufficiently fast (*i.e.*, $\overline{v} \geq 2C_0 + 1$).

In a physically more relevant model, there also might exist light particles with initial energies less than $2C_0+1$, equivalently, with initial velocities less than $m^{-1/2}(2C_0+1)$. We consider this case from now on. As explained, this could not be covered by [12] – the effective interaction time duration could not be bounded. Indeed, in a continuous interaction potential model with possibly not sufficiently fast light particles, the effective interaction time durations between particles might be unbounded. This is heuristically clear by considering the much simpler model with the massive particle frozen – if the initial relative position $x - X$ between a light particle and the frozen massive particle is parallel to its initial velocity v but with opposite directions, and the energy $\frac{m}{2}|v|^2 + U(x-X)$ is equal to the maximum of the potential U (which is assumed to be finite now), then after its first hit, the light particle will stop at the position that attains the maximum of the potential, hence the effective interaction time duration would be infinity.

For the model with light particles not sufficiently fast, we restrict ourselves to the case where the interactions between particles are repulsive. So we are assuming the following in addition:

U2. $h'(a) < 0$ for any $a \in (0, R_U)$. Also, we assume that $h''(0) < 0$.

In this case, at least for a light particle in a freezing-approximation model, as long as its initial relative position $x - X$ is not totally parallel to its initial velocity v, even if $|v| \le 2C_0 + 1$, the particle could leave the effective interaction range at some finite time. Certainly, the observation above suggests that the effective interaction time duration could nevertheless be very long. The situation for the light particles without freezing-approximation is even more complicated since the massive particle is also evolving.

By estimating the effective interaction time durations accurately, we can prove the following.

Theorem 3 ([14]) *Assume (U1) (U2) and (A1) $\sim$ (A3). Also, assume that $d > 2(1 + \|h''\|_\infty)(-h''(0))^{-\frac{1}{2}} + 1$. Then when $m \to 0$, the distribution of $\{(X^{(m)}(t), V^{(m)}(t));$
$t \ge 0\}$ under $\widetilde{P_m}$ converges weakly to the diffusion process with generator L in $(C([0,\infty); \mathbf{R}^{2d}), dist)$.*

We remark that the assumption $d > 2(1 + \|h''\|_\infty)(-h''(0))^{-1/2} + 1$ of Theorem 3 implies that $d > 5$. This assumption is closely related to our estimation of the effective interaction time durations of the light particles. It might by possible to relax this assumption if we can prove a sharper estimate.

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