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Probability Theory and Related Fields

Self-Diffusion in a Non-Uniform one Dimensional System of Point Particles with Collisions*

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Dedicated to Frank Spitzer on the occasion of his 60th birthday

Summary. We generalize the results of Spitzer, Jepsen and others [1–4] on the motion of a tagged particle in a uniform one dimensional system of point particles undergoing elastic collisions to the case where there is also an external potential $U(x)$. When $U(x)$ is periodic or random (bounded and statistically translation invariant) then the scaled trajectory of a tagged particle $y_A(t)=y(At)/\sqrt{A}$ converges, as $A\to\infty$, to a Brownian motion $W_D(t)$ with diffusion constant $D=\rho_{\min}\langle|v|\rangle/\hat{\rho}^2$, where $\hat{\rho}$ is the average density, $\langle|v|\rangle=\sqrt{2/\pi\beta m}$ is the mean absolute velocity and β^{-1} the temperature of the system. When $U(x)$ is itself changing on a macroscopic scale, i.e. $U_A(x)=U(x/\sqrt{A})$, then the limiting process is a spatially dependent diffusion. The stochastic differential equation describing this process is now non-linear, and is particularly simple in Stratonovich form. This lends weight to the belief that heuristics are best done in that form.

I. Introduction

The motion of a tagged (test) particle (tp) in an equilibrium fluid is one of the most studied problem in statistical mechanics [1–9]. It is a paradigm for extracting a (hopefully) simple stochastic description of the behavior of one component of a system with an enormously large number of degrees of freedom undergoing a complex deterministic evolution. The latter is for a classical fluid given by the Hamiltonian equations of motion while the former is known only approximately in the absence of some coarse graining [9]. We can achieve this by looking at the trajectories of the tp on a space and time scale

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which is very large (macroscopic) compared to the time scale on which the (microscopic) velocity of the tp changes. This is generally expected to yield a universal diffusive process in which the precise nature of the fluid interactions enter only through the diffusion constant.

An actual derivation of this expected result exists, despite the efforts of many, only for the simplest model systems. Chief among them is the fluid of hard rods or point particles on a line in which the tp is identical with (has the same mass as) the other particles [1–4]. In all these studies the fluid was taken to be spatially uniform so the resulting diffusion process was independent of the position of the tp. As a consequence there was no distinction between the Ito and Stratonovich prescription for the stochastic differential equation describing the process [10], i.e. we were dealing with a case of additive noise.

In the present work we consider (for the first time we believe) the case where the fluid is not spatially uniform in equilibrium. We show that the resulting process is still a diffusion but now inhomogeneous. The "noise" is therefore no longer additive and the stochastic differential equation describing the process now looks very different in its Ito or Stratonovich form. Interestingly we find that the Stratonovich form is definitely simpler – it involves no drift terms – and more natural. This gives weight to a general belief, which until now was based on very little rigorous evidence, that heuristic approximations are better done in the more symmetric Stratonovich form than in the mathematically simpler Ito form.

Model, Method, and Results

We consider an infinite system of identical point particles on the line moving in an external potential $U(x)$. The only interactions between the particles are elastic collisons, i.e. in a collision velocities are exchanged. These prevent particles from crossing, without affecting the infinite system motion if labeling is ignored. The particles are distributed according to the stationary grand canonical ensemble, i.e. their positions and velocities are Poisson with density $(\beta/2\pi)^{1/2}\rho_0 \exp\{-\beta[U(x)+\frac{1}{2}v^2]\}$.

As in [4] we study the asymptotics of the collision process of a tagged particle by relating its position at time t to the signed number $n(t)$ of crossings of the origin by particles before time t: $n(t)$ is the number of particles crossing the origin from left to right minus the number of particles crossing from right to left, which, of course, is the same as for the "free" motion, i.e. the motion without collisions.

To describe the essence of our approach consider first the much studied case $U \equiv 0$ [1, 4]. Then without collisions particles move in straight lines. As tagged particle we choose the first particle to the left of the origin at $t=0$. Following the path $y(t)$, $t \geqq 0$, of this particle (with collisions) one finds easily that

(i) $y(t)=x^t_{n(t)} \equiv$ the position of the $n(t)$-th particle to the right of the origin at time t.

Next observe that

(ii) $n(t)$, $t \geqq 0$, is a simple random walk with "± 1" jumps and jump rate $\rho\langle|v|\rangle$, where ρ is the density of the ideal gas and $\langle|v|\rangle$ the first absolute moment of the velocity distribution of the particles. This follows from the fact that in the free motion (a) particles can't cross the origin more than once and (b) in the ideal gas Gibbs state, which is stationary, "distinct particles are independent". Therefore $n(t)$, $t \geqq 0$, obeys the classical (functional) central limit theorem (Donsker's invariance principle) [11] with variance $\rho\langle|v|\rangle t$: the process $n(At)/\sqrt{A}$, $t \geqq 0$, converges in distribution as $A \to \infty$ to $Z(t)$, a Wiener process with diffusion constant $D_n = \rho\langle|v|\rangle$. Finally, for the ideal gas Gibbs state we have that

(iii) $x^t_{n(t)} \sim \rho^{-1} n(t)$ and therefore we obtain by (i) the invariance principle for $y(t)$, $t \geqq 0$, with variance $\rho^{-1}\langle|v|\rangle t$ [3]: $y(At)/\sqrt{A}$, $t \geqq 0$, converges in distribution to $\rho^{-1} Z(t)$, a Wiener process with diffusion constant $D_0 = \langle|v|\rangle/\rho$.

Now suppose the particles are moving in an external potential $U(x)$. Then the equilibrium density will be spatially varying: $\rho(x) = \rho_0 e^{-\beta U(x)}$ (β = inverse temperature). Just as for the case $U=0$, $y(t) = x^t_{n(t)}$, where $n(t)$, now the "crossing process" at the *maximum* of U (which we assume to be at the origin), obeys the invariance principle: $n(At)/\sqrt{A}$, $t \geqq 0$, converges in distribution to $Z(t)$, a Wiener process with diffusion constant $D_n = \rho_{\min}\langle|v|\rangle$, where $\rho_{\min}(=\rho(0)) = \rho_0 e^{-\beta U_0}$, $U_0 = \sup_x U(x)$. Moreover, if $U(x)$, $x \in \mathbb{R}$, is a (translate of) a simple of a translation invariant random bounded potential, then we have that $x^t_{n(t)} \sim \hat{\rho}^{-1} n(t)$ and hence that $y(At)/\sqrt{A}$, $t \geqq 0$, converges in distribution to $\hat{\rho}^{-1} Z(t)$, a Wiener process with diffusion constant $(\rho_{\min}/\hat{\rho})(\langle|v|\rangle/\hat{\rho}) = (\rho_{\min}/\hat{\rho}) D_0$, where $\hat{\rho} = \langle\rho\rangle$, the average density. This result does not, in fact, require full translation invariance, but merely that the "average density on the left" and on the right exist and agree, i.e. that the "macroscopic density" $\hat{\rho}$ be constant. If they do not agree, so that the macroscopic density $\hat{\rho}$ has different values on the left and on the right of the origin, it remains true that $x^t_{n(t)} \sim \hat{\rho}^{-1}(n(t))\, n(t)$ and hence that $y(At)/\sqrt{A}$, $t \geqq 0$, converges in distribution to $\hat{Z}(t) = \hat{\rho}^{-1}(Z(t))\, Z(t)$. $\hat{Z}(t)$ can be described by the stochastic differential equation $d\hat{Z} = (\hat{\rho}(\hat{Z}(t)))^{-1} \circ dZ$, provided that the differential is interpreted in the sense of Stratonovich [14].

We obtain the same result even if the potential varies on the macroscopic scale A: Let

$$U_A(x) = U(x/\sqrt{A}) \quad \text{and hence} \quad \rho_A(x) = \rho(x/\sqrt{A})$$

and consider now again the rescaled displacement of the test particle $y_A(t) = y(At)/\sqrt{A}$. As $A \to \infty$ the scale of the potential changes in just such a way as to make the external force on the tp, which is the same as that on any other fluid particle, have a finite nonvanishing effect over the macroscopic time scale At. Moreover, on the macroscopic scale the density varies as $\rho(x) = \rho_0 \cdot \exp[-\beta U(x)]$, i.e. the macroscopic density $\rho(x) = \rho(x)$ in this case.

Furthermore, since $n(t)$ is the number of particles between the origin and $y(t) = x^t_{n(t)}$, we should have that $dn = \rho_A\, dy$ and hence that $y(At)/\sqrt{A}$, $t \geqq 0$, converges in distribution to a process $\hat{Z}(t)$ satisfying $d\hat{Z}=\rho^{-1}(\hat{Z})\circ dZ$. This turns out to be correct, again provided the stochastic differential is interpreted in the sense of Stratonovich.

We thus obtain in the limit $A\to\infty$ the diffusion equation for the probability density of the tp $p(x,t)$ (x and t on macroscopic scale)

$$\frac{\partial p(x,t)}{\partial t}=\frac{1}{2}\frac{\partial}{\partial x}\left[-\beta D(x)K(x)p+D(x)\frac{\partial}{\partial x}p\right] \tag{1.1}$$

where $K(x)=-dU(x)/dx$, $D(x)=\rho_0\exp[-\beta U_0]\langle|v|\rangle\rho^{-2}(x)$ and the mobility $\beta D(x)$ satisfies the Einstein relation, as it must [11] for the equilibrium distribution to be a stationary solution of (1.1).

We conclude this section by noting the following consequence of the way the diffusion constant D depends upon the macroscopic density $\hat{\rho}$: *If* $U(x)$ is quasiperiodic then D exhibits sensitive dependence on the modulation parameters. For example, if $U(x)=\cos x+\cos kx$, then $D=D(k)=D^*$, independent of k, for k irrational and is unequal to D^* for k rational; in fact, D is continuous at all irrational k and discontinuous at rational k. These facts follow from the corresponding facts about $\hat{\rho}=\hat{\rho}(k)$. Similar results were discussed in [13] for diffusion in a quasiperiodic potential (Smoluchowski equation). Here the source of the discontinuity is perhaps more concrete since it lies in the density.

These results, for which we have just given heuristic arguments, are proven in the subsequent sections. The next section contains a detailed description of the model. In Sects. III and IV $n(t)$ and its asymptotics are studied. The corresponding results for the collision process $y(t)$ are then given in Sect. V.

II. The Free Motion

We consider an ideal gas of identical point particles moving in an external potential $U(x)$ and distributed according to the corresponding Gibbs state. We shall assume throughout the paper that

(2.1) $U(x)$ is bounded (and for convenience positive)

(2.2) $K(x)=-U'(x)$ is continuously differentiable

and

$$U(0)=U_0\equiv\sup_x U(x). \tag{2.3}$$

(2.1) is the key assumption. The existence and uniqueness of the motion considered below is ensured by (2.2) and (2.1), while (2.3) is a harmless but convenient condition, the role of which will become apparent later.

Let

$$(\underline{X},\underline{V})=(\{x_i^0\},\{v_i\}),\qquad x_i^0,\ v_i\in\mathbb{R},\ i\in\mathbb{Z},$$

specify the initial positions and velocities of the particles, labeled so that

$$\dots x_{-2}^0\leqq x_{-1}^0\leqq x_0^0\leqq 0<x_1^0\leqq x_2^0\leqq\dots.$$

The evolution of the system is given by the collection

$$(\underline{X}(t), \underline{V}(t))_{t \geqq 0} = (\{x_i(t)\}, \{v_i(t)\}),$$

where $x_i(t)$, $v_i(t)$ are the solution of the equations

$$\frac{dx_i(t)}{dt} = v_i(t)$$
$$\frac{dv_i(t)}{dt} = K(x_i(t)) \tag{2.4}$$

with $x_i(0) = x_i^0$ and $v_i(0) = v_i$.

The (invariant) Gibbs state of the system is conveniently described by a Poisson point process $(\Omega, \mathscr{F}, P)$ built over the phase space $\Gamma = \mathbb{R} \times \mathbb{R}$ with intensity

$$d\mu = (\beta/2\pi)^{\frac{1}{2}} \rho(x)\, e^{-\frac{1}{2}\beta v^2}\, dx\, dv, \qquad \rho(x) = \rho_0\, e^{-\beta U(x)}, \quad \rho_0 > 0, \tag{2.5}$$

where $\beta > 0$ is the inverse temperature and $dx\,dv$ is the Lebesgue measure on $\mathbb{R} \times \mathbb{R}$, using the natural identification of each point $\omega \in \Omega$ with a sequence $(\underline{X}, \underline{V})$.

Let T_t, $t \geqq 0$, denote the Newtonian flow on Γ given by the solution of (2.4). Then the mapping $\tau_t \colon \Omega \to \Omega$ given by

$$\omega = (\underline{X}, \underline{V}) \to \{T_t(x_i, v_i)\}_{i \in \mathbb{Z}} \equiv \omega_t$$

preserves P. In particular, the marginal distribution $P_x = P \circ \pi_x^{-1}$ is preserved, where π_x is the projection on the first component of ω.

III. The Collision Process

We now take elastic collisions between the particles into account: The trajectories of the "unlabeled" system remain unchanged, but the order of particles is preserved, i.e. particles cannot cross each other. This prescription agrees with the Newtonian evolution of the system with elastic collisions, i.e. when a two-particle-collision occurs the velocities of the colliding particles are simply exchanged.

We wish to observe the position $y(t)$, $t \geqq 0$, a random process on $(\Omega, \mathscr{F}, P)$, of a tagged particle. The simplest choice for tagged particle is the one starting at x_0^0. By our assumption (2.3) it is then also the first particle to the left of the absolute maximum of the potential U. We relabel $\underline{X}(t)$ and denote by $\{x_i^t\}$ the positions at time t, labeled in their natural order w.r.t. the origin, i.e.

$$\ldots x_{-2}^t \leqq x_{-1}^t \leqq x_0^t \leqq 0 < x_1^t \leqq x_2^t \ldots.$$

It is easy to see that when the tagged particle starts at x_0^0 our description of the collision process is equivalent to the following formula for $y(t)$:

$$y(t) = x_{n(t)}^t, \qquad t \geqq 0, \tag{3.1}$$

where $n(t)$ is the signed number of particles crossing the origin by time t (the "current" through the origin).

The essential point of the assumption (2.3) is that $U(x)$ achieve its supremum. The additional assumption that this is at the origin is made merely for convenience. We wish, however, to allow other possibilities for the choice of tagged particle (than the first particle to the left of the maximum of U). In general, instead of (3.1) we have that

(3.2) $$y(t)=x^t_{m(t)}, \qquad t \geqq 0,$$

where

(3.3) $$m(t)=n(t)+r$$

and r is the (possibly random) "index" of the tagged particle: the initial position of the tagged particle is x^0_r. r will be random, for example, if the tagged particle is the particle nearest a specified position q.

In the Smoluchowski case, in which U varies on the macroscopic scale, $U_A(x)=U(x/\sqrt{A})$, we wish also to allow for the possibility that the tagged particle is initially located near a specific position $q_A=q\sqrt{A}$ on the macroscopic scale. In this case $r \equiv r_A$ depends explicitly on A and satisfies

(3.4) $$r_A/\sqrt{A} \xrightarrow[A\to\infty]{} \bar{q}=\int_0^q \rho(x)\,dx.$$

We note in passing that, just as in [4], our main results are also valid when the tagged particle is an identical extra particle added to the system at a specific position.

IV. The Asymptotics of the Current $n(t)$

By conservation of the energy, $\frac{1}{2}v^2+U(x)$, particles can cross the origin (the absolute maximum of U) at most once. By the independence properties and time invariance of the Poisson field P we easily find that the mean current through the origin per unit time is zero and its variance is

(4.1) $$D_n=E(n(t)^2)/t=\rho_0\, e^{-\beta U_0}\sqrt{\beta/2\pi}\int_{-\infty}^{\infty}|v|\, e^{-\frac{1}{2}\beta v^2}\,dv$$
$$=\rho_0\, e^{-\beta U_0}\, E(|v|)$$

and that $n(t)$, $t\geqq 0$, is a continuous time simple symmetric random walk with jump rate D_n. Donsker's invariance principle immediately gives [11]

(4.2) **Proposition.** *Let*

$$n_A=(n_A(t))_{t\geqq 0}, \qquad n_A(t)=n(At)/\sqrt{A}.$$

Then n_A converges in distribution to $Z=\sqrt{D_n}\,W$ ($n_A \Rightarrow Z$), where W is a standard Wiener process.

V. The Asymptotics of $y(t)$

We introduce new coordinates

(5.1) $$\bar{x}=f(x)\equiv\int_0^x \rho(z)\,dz=\int_0^x \rho_0\, e^{-\beta U(z)}\,dz.$$

Since $d\bar{x}=\rho(x)\,dx$ and U is bounded

$$\bar{P}=P\circ F^{-1},$$

where

$$F:\Omega\to\Omega,\qquad F(\omega)=F(\underline{X},\underline{V})=\{f(x_i),v_i\},$$

is a Poisson measure with density on $\mathbb{R}^2$

$$d\bar{\mu}=d\bar{x}(\beta/2\pi)^{\frac{1}{2}}\,e^{-\frac{1}{2}\beta v^2}\,dv$$

and with spatial density 1.

Denoting by

$$\bar{\tau}_t=F\circ\tau_t\circ F^{-1}:\Omega\to\Omega$$

the "image of the Newtonian evolution τ_t under F", we have that

$$\bar{P}\circ\bar{\tau}_t^{-1}=P\circ F^{-1}\circ F\circ\tau_t^{-1}\circ F^{-1}=P\circ\tau_t^{-1}\circ F^{-1}=P\circ F^{-1}=\bar{P}$$

since $P\circ\tau_t^{-1}=P$, and in particular, that the marginal distribution $\bar{P}_x=\bar{P}\circ\pi_x^{-1}$, is preserved by $\bar{\tau}_t$.

We consider now the process (see Eq. (3.3))

(5.2) $$\bar{y}(t)=f(y(t))=\bar{x}^t_{m(t)},\qquad t\geqq 0.$$

(5.3) **Proposition.** *Let*

$$\bar{y}_A(t)=\bar{y}(At)/\sqrt{A},\qquad t\geqq 0.$$

Then for any $T<\infty$ and any $\delta>0$

$$\lim_{A\to\infty} P\Big(\sup_{t\in[0,T]}|\bar{y}_A(t)-m_A(t)|>\delta\Big)=0,$$

where $m_A(t)=m(At)/\sqrt{A}$.

Proof. The proof is the same as that of Proposition (3.1)(ii) of [3]. Roughly speaking one uses (5.2) and the stationarity of $\bar{P}$, noting that $\bar{x}^t_n/n\to 1$, $\bar{P}$ a.s., and that (in distribution) $|m(t)|\to\infty$ as $t\to\infty$, so that $\bar{x}^t_{m(t)}/m(t)\to 1$ as $t\to\infty$. The crucial step is to control the density fluctuations in the Poisson field $\bar{P}_x$ over a finite amount of time. For this, Condition (3.6) in [4] is needed. We leave it to the reader to verify that

(5.4) $$E\Big(\sup_{t\in[0,1]}\sup_x|\bar{x}_{x,v}(t)-\bar{x}|\Big)\leqq\rho_0\big(\sqrt{2U_0}+E|v|\big)<\infty.$$

replacing (3.6) in [4], ensures the Proposition (5.3).

To establish (5.4) let

$$\bar{x}_{x,v}(t)=f(x_{x,v}(t))$$

where $(x_{x,v}(t), v_{x,v}(t))$ satisfies (2.4) with $x(0)=x$ and $v(0)=v$, and note that

$$\bar{v}_{x,v}(t)=d\bar{x}_{x,v}(t)/dt=(dx_{x,v}(t)/dt)\,\rho(x_{x,v}(t))$$

and hence

$$|\bar{v}_{x,v}(t)|\leqq\rho_0(\sqrt{2U_0}+|v|), \qquad t\geqq 0$$

which proves (5.4).

By virtue of Proposition (4.2) we obtain from Proposition (5.3) [11]

(5.5) **Corollary.** *Let Z be as in Proposition* (4.2). *Then*

$$\bar{y}_A \Rightarrow Z.$$

V.1. Cesaro-mean Diffusions

Let $g\equiv f^{-1}$ where f is defined in (5.1). Then by (5.2)

$$y(t)=g(\bar{y}(t))$$

and

$$y_A(t)\equiv y(At)/\sqrt{A}=h_A(\bar{y}_A(t)),$$

where

(5.6) $$h_A(x)\equiv A^{-\frac{1}{2}}g(A^{\frac{1}{2}}x).$$

Clearly, $h_A\colon \mathbb{R}\to\mathbb{R}$ is continuous for all A. Suppose that

(5.7) h_A converges uniformly on compacts to a (continuous) function h.

Then, denoting by H_A, H the (sup-norm continuous) functions on $C[0,T]$, $T<\infty$, given by

$$H_A(\xi)=(h_A(\xi(t)))_{t\in[0,T]},$$

observe that for $y_A\equiv(y_A(t))_{t\in[0,T]}(\varepsilon C[0,T]$ for all $A)$

(5.8) $$y_A=H_A(\bar{y}_A)=H(\bar{y}_A)+(H_A(\bar{y}_A)-H(\bar{y}_A))\Rightarrow H(Z),$$

since H is continuous in the uniform topology on $C[0,T]$, and $h_A\to h$ uniformly on compacts while, by virtue of (5.5),

$$\lim_{B\to\infty} P(\sup_{[0,T]}\bar{y}_A(t)>B)=0$$

uniformly in A, so that $H_A(\bar{y}_A)-H(\bar{y}_A)\Rightarrow 0$.

Suppose again that (5.7) holds. Then by (5.6) h is homogeneous: $h(\gamma x)=\gamma h(x)$ for all $\gamma>0$. Thus $h(\pm\gamma)=\gamma h(\pm 1)$, i.e.

$$h(x)=\begin{cases} h(1)x & x\geqq 0\\ -h(-1)x & x\leqq 0\end{cases}$$

and in particular

(5.9)
$$\lim_{x\to\{{+\infty \atop -\infty}} \frac{1}{x} g(x) = \begin{cases} h(1) \\ h(-1) \end{cases}.$$

But $g=f^{-1}$ with $f(x)=\int_0^x \rho(z)\,dz$ and $\rho(z)$ uniformly bounded, so that (5.9) transforms easily to

(5.10)
$$\lim_{x\to\{{+\infty \atop -\infty}} \frac{1}{x} f(x) = \begin{cases} h(1)^{-1} \\ h(-1)^{-1} \end{cases}.$$

Note also that by the remark following (5.16), if $\lim y_A$ exists then (5.7) holds.

Conversely, suppose that

$$\lim_{x\to\{{+\infty \atop -\infty}} \frac{1}{x} f(x) = \begin{cases} \bar{\rho} \\ \underline{\rho} \end{cases} \text{ i.e. } \lim_{x\to\{{+\infty \atop -\infty}} \frac{1}{x} g(x) = \begin{cases} \bar{\rho}^{-1} \\ \underline{\rho}^{-1} \end{cases}.$$

Then (5.7) easily follows with

$$h(x) = \begin{cases} \bar{\rho}^{-1} x & x \geqq 0 \\ \underline{\rho}^{-1} x & x \leqq 0 \end{cases}.$$

We have thus proven

(5.11) **Theorem.** *Suppose that the following Cesaro limits exist:*

(5.12)
$$\lim_{L\to\infty} \frac{1}{L} \int_0^L e^{-\beta U(x)}\,dx \equiv \bar{\rho}/\rho_0$$
$$\lim_{L\to-\infty} \frac{1}{L} \int_0^L e^{-\beta U(x)}\,dx \equiv \underline{\rho}/\rho_0.$$

Then for Z as in Proposition (4.2)

(5.13)
$$y_A \Rightarrow \hat{Z} \equiv ((\hat{\rho}^{-1}(Z(t)))\,Z(t))_{t\geqq 0}$$

where

(5.14)
$$\hat{\rho}(x) = \begin{cases} \bar{\rho} & x \geqq 0 \\ \underline{\rho} & x < 0 \end{cases}.$$

Conversely, if $\lim y_A$ exists, it is of the form (5.13) and (5.12) holds. □

Remark. $\hat{Z}$ is a diffusion process formally given by the (Ito) stochastic differential equation (Ito's formula [14])

(5.15)
$$d\hat{Z} = \tfrac{1}{2}(\bar{\rho}^{-1} - \underline{\rho}^{-1})\,D_n\,\delta(\hat{\rho}(\hat{Z}(t))\,\hat{Z}(t))\,dt + \hat{\rho}^{-1}(\hat{Z}(t))\sqrt{D_n}\,dW(t),$$

where $\hat{\rho}$ is defined after (5.13). If Stratonovich differentials are formally used instead, the equation for $\hat{Z}$ simplifies,

(5.16)
$$d\hat{Z} = \hat{\rho}^{-1}(\hat{Z})\sqrt{D_n} \circ dW,$$

since the ordinary rules of calculus apply to Stratonovich integrals.

Remark. We remark that for a general U, not necessarily satisfying (5.12), the family $\{h_A\}_{A\geqq 1}$ is compact in the topology of uniform convergence on compacts, by the Arzela Ascoli Theorem. To see this note that $|dh_A(x)/dx| \leqq e^{\beta U_0}$ uniformly in A and x, and that $h_A(0)=0$. Therefore if (5.7) is not satisfied, then there exist subsequences A_n and $\tilde{A}_n$ on which different limits h and $\tilde{h}$ are obtained and hence different limiting processes $h(Z)$ and $\tilde{h}(Z)$.

V.2. Smoluchowski-type Limits

We now consider potentials $U_A(x)$ which vary on the macroscopic scale, i.e.

(5.17) $$U_A(x) = U(x/A^{\frac{1}{2}})$$

(with U still satisfying (2.1)–(2.3)).

Therefore we have to replace $\rho(x)$ $(=\rho_0 \exp(-\beta U(x)))$ by $\rho_A(x)=\rho(x/A^{\frac{1}{2}})$ and thus the Poisson field $(\Omega, \mathcal{F}, P_A)$ becomes A-dependent. Slightly abusing notations we use again n_A, y_A and $\bar{y}_A$ for the processes now defined on $(\Omega, \mathcal{F}, P_A)$.

The reader may easily check that all results prior to Sect. V.1 are valid when P is replaced by P_A, provided Z in Corollary (5.5) is replaced by $Z_{\bar{q}}=Z+\bar{q}$, a Wiener process starting at $\bar{q}$; cf. Eq. (3.4). (In Proposition (5.3) $m(t)=n(t)+r_A$.) Moreover, it is now very simple to obtain the asymptotics of y_A from (5.5).

We have that

$$y_A = h_A(\bar{y}_A) \quad \text{where } h_A(\cdot) = \frac{1}{\sqrt{A}} f_A^{-1}(\sqrt{A}\,\cdot)$$

with

$$f_A(x) = \int_0^x \rho_A(z)\,dz = \int_0^x \rho\left(\frac{z}{\sqrt{A}}\right) dz = \sqrt{A}\, f(\sqrt{A}^{-1} x).$$

But

$$f_A^{-1}(x) = \sqrt{A}\, f^{-1}(\sqrt{A}^{-1} x)$$

and therefore

$$h_A(\cdot) = f^{-1}(\cdot) = g(\cdot)$$

so that in fact

(5.18) $$y_A = g(\bar{y}_A).$$

We thus obtain

(5.19) **Theorem.** *Suppose that U_A varies on the macroscopic scale (Eq. (5.17)). Then*

(5.20) $$y_A \Rightarrow \hat{Z} \equiv (g(Z(t)+\bar{q}))_{t\geqq 0},$$

where g is the inverse of the function $x \to \int_0^x \rho(y)\,dy$, with $\rho=\rho_0\, e^{-\beta U(x)}$, and where $\bar{q}$ is related to the initial position of y_A via Eq. (3.4). (Z is as in Proposition (4.2)).

$\hat{Z}$ is a diffusion process given by the stochastic differential equation

$$(5.21)\qquad d\hat{Z}(t) = -\tfrac{1}{2}\beta K(\hat{Z}(t))\, D_n\, \rho(\hat{Z}(t))^{-2}\, dt + \sqrt{D_n}\, \rho(\hat{Z}(t))^{-1}\, dW(t)$$

with $\hat{Z}(0)=q$. Using Stratonovich differentials

$$(5.22)\qquad d\hat{Z} = \rho(\hat{Z}(t))^{-1} \sqrt{D_n} \circ dW(t).$$

Proof. (5.20) follows from (5.5) using (5.18) and the fact that g is continuous [11].

(5.21) follows from Ito's formula and the observation that $g=f^{-1}$ so that by (5.1)

$$dg(x)/dx = \rho(g(x))^{-1}$$

and

$$\begin{aligned} d^2 g(x)/dx^2 &= -\rho(g(x))^{-3} (d\rho(x)/dx)_{g(x)} \\ &= -\beta K(g(x))\, \rho(g(x))^{-2} \end{aligned}$$

while (5.22) follows from the fact that the ordinary rules of calculus, in particular the chain rule, are valid for Stratonovich integrals. □

Remark. The Fokker-Planck (forward) generator corresponding to $\hat{Z}$ is

$$L = -(d/dx)\, b + \tfrac{1}{2}(d^2/dx^2)\, D(x)$$

and written in a "diffusion symmetric" form

$$L = -(d/dx)(b - \tfrac{1}{2} dD(x)/dx) + \tfrac{1}{2}(d/dx)\, D(x)(d/dx)$$

with

$$b(x) = -\tfrac{1}{2}\beta K(x)\, D_n\, \rho(x)^{-2}$$

and

$$D(x) = D_n\, \rho(x)^{-2}.$$

Noting that

$$b(x) - \tfrac{1}{2} dD(x)/dx = \tfrac{1}{2}\beta K(x)\, D(x)$$

we obtain that

$$L = -(d/dx)(\tfrac{1}{2}\beta K(x)\, D(x) - \tfrac{1}{2} D(x)\, d/dx)$$

and we easily read off that $L\rho(x)=0$, i.e. $\rho(x)=\rho_0\, e^{-\beta U(x)}$ is a stationary distribution for $\hat{Z}$. We may also recognize in this "diffusion symmetric" form of L the Einstein relation between the "mobility" $v(x)=\tfrac{1}{2}\beta D(x)$ and the Diffusion coefficient $D(x)$. Note that the usual form of the generator suggests an "anti-Einstein relation", since $b(x) = -v(x)\, K(x)$ so that $b(x)$ and $D(x)$ are related by an Einstein relation with a minus sign.

Remark. The fact that $\hat{Z}$ is most simply expressed as a Stratonovich integral can be understood in terms of symmetry properties under time reversal: $n(t)$ and $\int \rho(\hat{Z})^{-1} \circ dZ$ are both antisymmetric.

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