

Adiabatic Elimination for Systems of Brownian Particles with Nonconstant Damping Coefficients

J. M. Sancho,¹ M. San Miguel,¹ and D. Dürr²

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We discuss the problem of eliminating the momentum variable in the phase space Langevin equations for a system of Brownian particles in two related situations: (i) position-dependent damping and (ii) existence of hydrodynamic interactions. We discuss the problems associated with the conventional elimination and we develop an alternative elimination procedure, in the Langevin framework, which leads to the correct Smoluchowski equation. We give a heuristic argument on the basis of stochastic differential equations for the Smoluchowski limit and establish rigorously the limit for the general case of position-dependent friction and diffusion coefficients.

KEY WORDS: Adiabatic elimination; Langevin equation; stochastic equations; Fokker-Planck equation; Brownian motion, Smoluchowski approximation.

1. INTRODUCTION

The elimination of slow or irrelevant variables is a usual procedure to deal with macroscopic systems. Such a contraction of the description is a central idea of statistical mechanics. From a microscopic point of view several schemes (mostly based on projector formalisms) have been developed to derive equations describing a macroscopic behavior from the detailed mechanics of the individual components of the system. From a more phenomenological point of view one often faces a set of equations for a few variables which evolve in well-differentiated time scales. The adiabatic elimination⁽¹⁾ of the fast variables leads to a simpler description of the

¹ Departamento de Física Teórica, Universidad de Barcelona, Diagonal 647, Barcelona-28, Spain.

² Hill Center for the Mathematical Sciences, Rutgers University, New Brunswick, New Jersey 08903, USA.

system valid on the slowest time scale. One of the simplest examples of this elimination of variables is the passage from a phase space description of a Brownian particle to a description in terms of its position⁽²⁾ only.

A usual phenomenological description of a great variety of systems features a set of nonlinear coupled Langevin equations with Gaussian white noise random forces. The "conventional" adiabatic elimination consists in setting the time derivative of the fast variables equal to zero. In this way these variables are assumed to follow instantaneously the slow variables acquiring a constrained stationary value. This conventional adiabatic elimination is believed to represent in some sense a zeroth-order approximation. Corrections to this approximation take into account the finite relaxation time of the fast variables. An alternative approach to this procedure is the elimination of variables from the Fokker-Planck equation equivalent to the starting set of Langevin equations. In a previous paper⁽²⁾ two of the authors discussed the elimination of the momentum in the Langevin equations describing noninteracting Brownian particles. The major difficulty there was to deal with the non-Markovian Langevin equation obtained after the elimination of the velocity. A second difficulty that can arise in eliminating variables in Langevin equations is the appearance of terms which are nonlinear in the random forces. This problem can be handled with the approximation developed in a different context in Ref. 3.

In the case of Brownian particles without hydrodynamic interactions⁽²⁾ the conventional adiabatic elimination leads to the correct zeroth-order approximation which is known as the Smoluchowski approximation. This procedure might lead to ambiguities when the random force driving the system is not independent of the variables of the system (multiplicative noise). This occurs for Brownian particles with hydrodynamic interactions, where the random force is position dependent. These ambiguities in the conventional adiabatic elimination, without explicit reference to this particular system, have already been recognized.⁽⁴⁻⁷⁾ The difficulty has been traced back⁽⁴⁻⁶⁾ to the nonunique interpretation of the Langevin equation in position space which results after elimination of the momentum. In Sections 2 and 3 of this paper we rederive the correct zeroth-order approximation (Smoluchowski limit) in the problem of eliminating the momenta in the Langevin equations for a system of Brownian particles with hydrodynamic interactions. We do not make any reference to the Itô or Stratonovich interpretation^(8,9,20) of the Langevin equations involved: we use the Langevin equations and ordinary calculus and switch before going to the limit of infinite friction coefficient to the equation for the probability density of the positions. In the limit we thus end up with the Fokker-Planck equation for the problem, which of course uniquely defines the position process. In this section we follow the main ideas of Ref. 2. For

clarity of presentation we discuss first in Section 2 the simpler problem of a one-dimensional Brownian particle with position-dependent damping. In higher dimensions one may proceed similarly and in Section 3 we quote the result for Brownian particles with hydrodynamic interactions. The first two sections do not establish in a rigorous way the Smoluchowski limit of the problem. They rather represent a “physical” approach to the correct limit equation. This is done in Sections 4 and 5, which are more mathematical in nature. There, the Smoluchowski limit is obtained by using stochastic differential equations. We first give a mathematically heuristic argument for the limit equation obtained in Section 2, using the Stratonovich and Itô definitions of the stochastic integrals. We then establish the convergence of the position process to the limiting process in a specified sense.

From a microscopic point of view the problem of the Smoluchowski approximation in this context was discussed by Murphy and Aguirre⁽¹⁰⁾ and from a phenomenological Fokker–Planck point of view by Wilemski⁽¹¹⁾ and Titulaer.⁽¹²⁾ Related work from the Fokker–Planck perspective is due to Ryter,⁽⁴⁾ Risken *et al.*,⁽³⁾ Kaneko,⁽¹⁴⁾ and Gavish.⁽¹⁵⁾ From the Langevin perspective that we follow in Section 2 the work of Hess and Klein⁽¹⁶⁾ is similar in spirit but different in form from ours, while Hesegawa *et al.*⁽⁵⁾ discuss the general problem of elimination of variables along the lines of Section 4. The examples considered in Ref. 17 do not include the case of adiabatic elimination from Langevin equations with multiplicative noise.

2. POSITION-DEPENDENT FRICTION

In this section we consider an independent one-dimensional Brownian particle moving in a potential $\phi(q)$ and in a nonhomogeneous medium such that the friction coefficient $\lambda(q)$ is position dependent.^(4,5,6,13) The equations of motion for the momentum p and position q of the Brownian particle are

$$\dot{q}(t) = p(t) \quad (2.1)$$

$$\dot{p}(t) = -\lambda(q(t))p(t) - \phi'(q(t)) + g(q(t))\xi(t) \quad (2.2)$$

where ϕ' means the derivative of ϕ with respect to q and the random force $\xi(t)$ is assumed to be Gaussian white noise with zero mean and correlation

$$\langle \xi(t)\xi(t') \rangle = 2\delta(t - t') \quad (2.3)$$

The fluctuation dissipation theorem relates $g(q)$ and $\lambda(q)$ by

$$g^2(q) = K_B T \lambda(q) \quad (2.4)$$

where K_B is the Boltzmann constant and the temperature T may also depend on q . This relation is obtained imposing that the Fokker–Planck

equation in phase space, equivalent to (2.1)–(2.2), has the correct equilibrium solution. In what follows we do not require (2.4) to hold. The momentum p can be considered a fast variable under the assumption of a large damping coefficient $\lambda(q)$. [$\lambda(q) \geq \lambda_0$ and λ_0 is a large number.] The elimination of p should then give rise to an equation for the probability density $P(q, t)$ in position space. The exact equation satisfied by $P(q, t)$ is difficult to obtain even in much simpler situations.⁽²⁾ Therefore what one aims at in general is to obtain the leading terms of such an equation in an expansion in powers of $\lambda^{-1}(q)$. The conventional adiabatic elimination which in general is assumed to give the correct zeroth-order approximation consists in setting $p = 0$ in (2.2) and substituting in (2.1). This results in a stochastic equation in position space with position-dependent random term (“multiplicative noise”). It is therefore necessary to give an interpretation of that equation. In doing so one might run into problems if one considers a case in which (2.4) holds. The equation considered as Stratonovich as well as Itô^(8,9) does not give the correct answer, as might be seen from its stationary solutions, which are not correct equilibrium distribution $P_{\text{eq}} = N \exp[-\phi(q)/k_B T]$. How the limit has to be looked at is the subject of Section 4.

To eliminate p we shall then follow the method we introduced in the case of constant damping.⁽²⁾ The first step is the formal integration of (2.2) obtaining

$$\begin{aligned} \dot{q}(t) = p(t) = & - \int_0^t \exp \left[- \int_s^t \lambda(q(t')) dt' \right] \phi(q(s)) ds \\ & + \int_0^t \exp \left[- \int_s^t \lambda(q(t')) dt' \right] g(q(s)) \xi(s) ds \end{aligned} \quad (2.5)$$

where we have neglected transient terms involving the initial momentum. The two terms on the right-hand side of (2.5) are, respectively, of order λ^{-1} and $\lambda^{-1/2}$, as can be seen from (2.3) and because the time integral of $\exp - \int_s^t \lambda(q(t')) dt'$ is of order λ^{-1} . To simplify the memory kernels in (2.5) we expand $\lambda(q(t'))$ as

$$\lambda(q(t')) = \lambda(q(t)) - \frac{d\lambda(q(t))}{dq(t)} (q(t) - q(t')) + \dots \quad (2.6)$$

where $q(t) - q(t')$ is expressed from (2.5) as

$$\begin{aligned} q(t) - q(t') = & - \int_{t'}^t ds' \int_0^{s'} \exp \left[- \int_s^{s'} \lambda(q(t'')) dt'' \right] \phi'(q(s)) ds \\ & + \int_{t'}^t ds' \int_0^{s'} \exp \left[- \int_s^{s'} \lambda(q(t'')) dt'' \right] g(q(s)) \xi(s) ds \end{aligned} \quad (2.7)$$

The two terms on the right-hand side of (2.7) are, respectively, of order λ^{-2} and $\lambda^{-3/2}$. Substituting (2.7) in (2.6) we have

$$\begin{aligned} \lambda(q(t')) &= \lambda(q(t)) - \frac{d\lambda(q(t))}{dq(t)} \int_{t'}^t ds' \\ &\quad \times \int_0^{s'} \exp\left[-\int_s^{s'} \lambda(q(t'')) dt''\right] g(q(s)) \xi(s) ds + O(\lambda^{-1}) \\ &= \lambda(q(t)) + O(\lambda^{-1/2}) \end{aligned} \quad (2.8)$$

so that

$$\exp\left[-\int_s^t \lambda(q(t')) dt'\right] = \exp[-\lambda(q(t))(t-s)] \cdot [1 + O(\lambda^{-1/2})] \quad (2.9)$$

The result in (2.8) coincides with one in Ref. 7 and characterizes the effect of a position-dependent friction. In our case a more important effect comes from the existence of multiplicative noise. This effect of $g(q)$ is analyzed expanding $g(q(s))$ as we did above with $\lambda(q(t'))$. We obtain

$$\begin{aligned} g(q(s)) &= g(q(t)) - \frac{dg(q(t))}{dq(t)} \cdot g(q(t)) \int_s^t dt' \\ &\quad \times \int_0^{t'} \exp[-\lambda(q(t))(t'-s')] \xi(s') ds' + O(\lambda^{-3/2}) \end{aligned} \quad (2.10)$$

and similarly

$$\phi'(q(s)) = \phi'(q(t)) + O(\lambda^{-3/2}) \quad (2.11)$$

Substituting (2.9), (2.10), and (2.11) in (2.5) we have

$$\begin{aligned} \dot{q}(t) &= -\frac{\phi'(q(t))}{\lambda(q(t))} + g(q(t)) \int_0^t e^{-\lambda(q(t))(t-s)} \xi(s) ds \\ &\quad - \frac{dg(q(t))}{dq(t)} \cdot g(q(t)) \int_0^t e^{-\lambda(q(t))(t-t')} \xi(t') dt' \\ &\quad \times \int_{t'}^t ds \int_0^s e^{-\lambda(q(t))(s-s')} \xi(s') ds' + O(\lambda^{-3/2}) \end{aligned} \quad (2.12)$$

This is our basic stochastic equation in position space from which we shall derive the equation for the probability density $P(q, t)$. There are two origins of complexity in this stochastic equation. The first is the appearance of nonwhite random forces due to the time integrals on the right-hand side of (2.12). This is fundamentally the same problem that appears for constant

friction⁽²⁾ (see also Ref. 7). The second is the nonlinear form in which the random force $\xi(s)$ appears in the third term of the right-hand side of (2.12). The presence of this third term is due to the multiplicative character of the noise [$g(q)$ nonconstant].

The second term on the right-hand side of (2.12) can be interpreted in terms of a nonwhite or colored random force

$$\bar{\xi}(t) = \int_0^t e^{-\lambda(q(t))(t-s)} \xi(s) ds \tag{2.13}$$

which in leading order in λ^{-1} can be approximated⁽²⁾ by a Gaussian white noise

$$\bar{\xi}(t) \simeq \frac{\xi(t)}{\lambda(q(t))} + O(\lambda^{-2}) \tag{2.14}$$

The last term in (2.12) is more complicated and a way to handle it is through the stochastic Liouville equation⁽¹⁸⁾ for the density $\rho(q, t)$ of an ensemble of representative points obeying (2.12). Taking the average over the stochastic force $\xi(t)$ we obtain a formal master equation for the probability density of the process $P(q, t) = \langle \rho(q, t) \rangle$

$$\begin{aligned} \frac{\partial P(q, t)}{\partial t} &= \frac{\partial}{\partial q} \frac{\phi'(q)}{\lambda(q)} P(q, t) - \frac{\partial}{\partial q} \frac{g(q)}{\lambda(q)} \langle \xi(t) \rho(q, t) \rangle \\ &+ \frac{\partial}{\partial q} \frac{dg(q)}{dq} \cdot g(q) \int_0^t e^{-\lambda(q)(t-t')} dt' \\ &\times \int_{t'}^t ds \int_0^s e^{-\lambda(q)(s-s')} ds' \langle \xi(t') \xi(s') \rho(q, t) \rangle \end{aligned} \tag{2.15}$$

The statistical averages in (2.15) can be performed using the functional characterization of Gaussian forces due to Novikov⁽¹⁹⁾: with $\xi(t)$ being a white noise we have⁽²⁾

$$\langle \xi(t) \rho(q, t) \rangle = - \frac{\partial}{\partial q} \frac{g(q)}{\lambda(q)} P(q, t) + O(\lambda^{-2}) \tag{2.16}$$

and generalizing Novikov's theorem to deal with a nonlinear term in $\xi(t)$ ⁽³⁾:

$$\langle \xi(t') \xi(s') \rho(q, t) \rangle = 2\delta(t' - s') P(q, t) + \left\langle \frac{\delta^2 \rho(q, t)}{\delta \xi(s') \delta \xi(t')} \right\rangle \tag{2.17}$$

The last term in (2.17) will contribute in higher orders in λ^{-1} when it is substituted in (2.15). Neglecting this term and substituting in (2.15) we

arrive at the following Fokker–Planck equation:

$$\begin{aligned} \frac{\partial P(q, t)}{\partial t} = & \frac{\partial}{\partial q} \frac{\phi'(q)}{\lambda(q)} P(q, t) + \frac{\partial}{\partial q} \frac{g(q)}{\lambda(q)} \frac{\partial}{\partial q} \frac{g(q)}{\lambda(q)} P(q, t) \\ & + \frac{\partial}{\partial q} \frac{1}{\lambda(q)^2} \frac{dg(q)}{dq} g(q) P(q, t) \end{aligned} \quad (2.18)$$

which can be written in the case of (2.4) as

$$\frac{\partial P(q, t)}{\partial t} = \frac{\partial}{\partial q} \frac{1}{\lambda(q)} \left[\phi'(q) + k_B T \frac{\partial}{\partial q} \right] P(q, t) \quad (2.19)$$

This equation represents the Smoluchowski approximation to the problem³ and has the correct equilibrium distribution $P_{\text{eq}}(q) = Ne^{-\phi(q)/k_B T}$. Of course the usefulness of this equation is not to obtain the equilibrium distribution but to obtain, for instance, a stationary distribution under given nonequilibrium conditions.

From equation (2.18) we can write an equivalent stochastic equation which in the ordinary Stratonovich interpretation is

$$\dot{q} = -\frac{\phi'(q)}{\lambda(q)} - \frac{1}{\lambda(q)^2} g'(q) g(q) + \frac{g(q)}{\lambda(q)} \xi(t) \quad (2.20)$$

This equation differs from the one obtained in the conventional adiabatic elimination in the presence of the second term on the right-hand side. This term represents the effect of the multiplicative character of the noise in the elimination procedure and it is just the average of the third term on the right-hand side of (2.12). This fact justifies a posteriori the substitution (in leading order) of such an awkward term in (2.12) by its mean value.⁽¹⁶⁾

3. SMOLUCHOWSKI EQUATION FOR BROWNIAN PARTICLES WITH HYDRODYNAMIC INTERACTIONS

The equations of motion are in this case

$$\dot{q}_i(t) = p_i(t) \quad (3.1)$$

$$\dot{p}_i(t) = -\lambda_{ij}(|q_i - q_j|) p_j(t) - \phi_i(q) + g_{ij}(q) \xi_j(t) \quad (3.2)$$

where

$$\phi_i(q) = \frac{\partial}{\partial q_i} \phi(\mathbf{q}, \dots, \mathbf{q}_N) \quad (3.3)$$

³ Starting from the Fokker–Planck equation in phase space, the first correction to (2.19) has been obtained by Risken *et al.*⁽¹³⁾ using the matrix continued fraction expansion.

and the indexes i, j refer both to different particles and different vector components of the momentum and position. The quantity $\lambda_{ij}(|q_i - q_j|)$ is the generalized friction tensor which represents the hydrodynamic interaction between two particles. The elements of λ_{ij} corresponding to the same particle are self-friction constant coefficients.

The random forces are Gaussian white noise with zero mean and correlation

$$\langle \xi_i(t) \xi_j(t') \rangle = 2\delta_{ij} \delta(t - t') \quad (3.4)$$

and the fluctuation dissipation relation is

$$g_{ik} g_{jk} = k_B T \lambda_{ij} \quad (3.5)$$

where in (3.5) and in the following we do not make explicit the dependence on the position variables.

The Smoluchowski approximation for this problem can be obtained following step by step the procedure of the previous section. We only quote here the results. The stochastic equation analogous to (2.10) in the average of the equation corresponding to (2.12) and it is

$$\dot{q}_i(t) = -\lambda_{ie}^{-1} \phi_e - \frac{\partial g_{ej}}{\partial q_k} \cdot g_{mj} \lambda_{ie}^{-1} \lambda_{km}^{-1} + \lambda_{ie}^{-1} g_{ej} \xi_j(t) \quad (3.6)$$

From this equation the Fokker-Planck equation corresponding to the Smoluchowski approximation becomes⁴

$$\frac{\partial P(\mathbf{q}, t)}{\partial t} = \frac{\partial}{\partial q_i} \lambda_{ie}^{-1} \left(\phi_e + k_B T \frac{\partial}{\partial q_e} \right) P(\mathbf{q}, t) \quad (3.7)$$

4. A HEURISTIC ARGUMENT

Let us write the equations (2.1) and (2.2) as stochastic differential equations in the form⁽²⁰⁾

$$dq(t) = p(t) dt \quad (4.1)$$

$$dp(t) = \beta k(q(t)) dt - \beta \gamma(q(t)) p(t) dt + \beta \delta(q(t)) dW_t \quad (4.2)$$

$\beta > 0$, $\gamma(q) > \gamma > 0$, and $\delta(q) > 0$.

Here W_t is the Wiener process with variance $E(W_t^2) = t$ and $E(\cdot)$ denotes the expectation. Note that $\beta K = -\phi'$; $\beta \gamma = \lambda$ and because of (2.3)

⁴ The first correction to this equation for a particular case has been obtained by Titulaer⁽¹²⁾ starting from the Fokker-Planck equation in phase space.

$\beta\delta = \sqrt{2} g$. By adiabatic elimination ($dp(t)/\beta = 0$ for $\beta \rightarrow \infty$) we obtain

$$dq(t) = \frac{K(q(t))}{\gamma(q(t))} dt + \frac{\delta(q(t))}{\gamma(q(t))} dW_t$$

Since the new diffusion coefficient δ/γ is position dependent one has to specify the meaning of the stochastic differential dW_t . The appropriate interpretation follows from a simple heuristic argument.

Inserting (4.1) in (4.2) we obtain

$$\frac{dp(t)}{\beta} = K(q(t)) dt - \gamma(q(t)) dq(t) + \delta(q(t)) dW_t \tag{4.3}$$

We write (4.3) as an integral equation

$$\int_0^t \frac{dp(s)}{\beta} = \int_0^t K(q(s)) ds - \int_0^t \gamma(q(s)) dq(s) + \int_0^t \delta(q(s)) dW_s \tag{4.4}$$

Without making precise the sense of convergence, we can see that as $\beta \rightarrow \infty$ and $q(t) \rightarrow \hat{q}(t)$ the following will occur:

- (i) The integral $\int_0^t K(q(s)) ds$ will converge to the time integral $\int_0^t K(\hat{q}(s)) ds$.
- (ii) The integral $\int_0^t \gamma(q(s)) dq(s)$ will converge to a Stratonovich stochastic integral

$$\int_0^t \gamma(\hat{q}(s)) \circ d\hat{q}(s)$$

by the theorem of Wong and Zakai,⁽²⁰⁾ which roughly says that the stochastic integral as a limit of Stieltjes integrals is a Stratonovich integral.

- (iii) The integral $\int_0^t \delta(q(s)) dW_s$ will converge to the Itô integral

$$\int_0^t \delta(\hat{q}(s)) dW_s \tag{4.5}$$

for the following reason. For finite β we have that

$$E\left(\int_0^t \delta(q(s)) dW_s\right) = 0$$

which should then also hold true for the limit, i.e., (4.5) will be an Itô integral.

Thus we obtain from (4.4)

$$0 = K(\hat{q}(s)) ds - \gamma(\hat{q}(s)) \circ d\hat{q}(s) + \delta(\hat{q}(s)) dW_s$$

and transforming the Stratonovich differential into an Itô differential⁽²⁰⁾

$$0 = K(\hat{q}(s)) ds - \gamma(\hat{q}(s)) d\hat{q}(s) - \frac{1}{2} \gamma'(\hat{q}(s)) (d\hat{q}(s))^2 + \delta(\hat{q}(s)) dW_s$$

where

$$\gamma'(x) = \frac{d}{dx} \gamma(x)$$

Solving for $d\hat{q}(s)$ we obtain

$$d\hat{q}(s) = \frac{K(\hat{q}(s))}{\gamma(\hat{q}(s))} - \frac{1}{2} \frac{\gamma'(\hat{q}(s))}{\gamma(\hat{q}(s))} [d\hat{q}(s)]^2 + \frac{\delta(\hat{q}(s))}{\gamma(\hat{q}(s))} dW_s$$

and find

$$(d\hat{q}(s))^2 = \frac{\delta^2(\hat{q}(s))}{\gamma^2(\hat{q}(s))} ds$$

so that finally

$$d\hat{q}(s) = \frac{K(\hat{q}(s))}{\gamma(\hat{q}(s))} ds - \frac{1}{2} \frac{\gamma'(\hat{q}(s))}{\gamma^3(\hat{q}(s))} \delta^2(\hat{q}(s)) ds + \frac{\delta(\hat{q}(s))}{\gamma(\hat{q}(s))} dW_s \quad (4.6)$$

The limit process $\hat{q}(t)$ satisfying (4.6) is the one derived in Section 2. Indeed converting (2.20) into an Itô equation and doing the proper identification gives (4.6).

We see that the adiabatic elimination on the level of Langevin equations works also for the case where the drift and diffusion coefficients are position dependent provided some care with stochastic differential is exercised.

At the heuristic level of this section it is interesting to note that the difficulties encountered in (2.12) because of the appearance of a nonlinear function of a white noise have been here bypassed through the appearance of $[d\hat{q}(s)]^2$ in an Itô equation.

We do not know of any rigorous proof for (4.6) to be the limit stochastic differential equation of the limit of $q(t)$ as $\beta \rightarrow \infty$. Nelson⁽²¹⁾ proves that in case for $\gamma = \text{const}$ and $\delta = \text{const}$ the process $q(t)$ converges almost certainly to $\hat{q}(t)$, where in view of (4.6)

$$d\hat{q}(t) = \frac{K(\hat{q}(t))}{\gamma} dt + \frac{\delta}{\gamma} dW_t$$

In the next section we extend his proof but we only show convergence in the L^2 sense. Therefore our theorem is only a weak extension of Nelson's theorem.

5. A CONVERGENCE THEOREM

Let $\gamma(z) \geq a > 0$ be such that

$$y = \Gamma(x) = \int_0^x \gamma(z) dz \quad (5.1)$$

is invertible and let $\Gamma^{-1}(y)$, $\bar{K}(y) = K \circ \Gamma^{-1}(y)$, $\bar{\delta}(y) = \delta \circ \Gamma^{-1}(y)$ be globally Lipschitz with Lipschitz constants A, B, C , i.e.,

$$|\Gamma^{-1}(y) - \Gamma^{-1}(y')| \leq A|y - y'| \quad (5.2)$$

$$|\bar{K}(y) - \bar{K}(y')| \leq B|y - y'| \quad (5.3)$$

$$|\bar{\delta}(y) - \bar{\delta}(y')| \leq C|y - y'| \quad (5.4)$$

Let $q(t)$ be the solution of

$$dq(t) = p(t) dt, \quad q(0) = q_0 \quad (5.5)$$

$$dp(t) = \beta K(q(t)) dt - \beta \gamma(q(t)) p(t) dt - \beta \delta(q(t)) dW_t \quad (5.6)$$

$$p(0) = p_0$$

and $\hat{q}(t)$ the solution of the (Itô) stochastic differential equation (4.6) with $\hat{q}(0) = q(0) = q_0$.

Then for $t \in [0, \infty)$

$$\lim_{\beta \rightarrow \infty} E((q(t) - \hat{q}(t))^2) = 0 \quad (5.7)$$

Proof. Let $y(t) = \Gamma(q(t))$, then with (5.5)

$$dy(t) = \gamma(q(t)) p(t) dt, \quad y(0) = \Gamma(q_0)$$

and combining this with (5.6) we obtain

$$dy(t) = -\frac{dp(t)}{\beta} + \bar{K}(y(t)) dt + \bar{\delta}(y(t)) dW_t, \quad y(0) = \Gamma(q_0) \quad (5.8)$$

For $n \in N$ we define the time interval $\Delta_n = [t_n, t_{n+1}]$ of length $|\Delta_n|$ such that

$$16|\Delta_n|^2 B^2 + 16|\Delta_n| C^2 = 1/2 \quad (5.9)$$

For $t \in \Delta_n$ we obtain from (5.8)

$$y(t) - y(t_n) = -\frac{1}{\beta} [p(t) - p(t_n)] + \int_{t_n}^t \bar{K}(y(s)) ds + \int_{t_n}^t \bar{\delta}(y(s)) dW_s \quad (5.10)$$

Since (5.6) is linear in the velocity, $p(t)$ can be found very easily as a function of $q(t)$:

$$\begin{aligned} \frac{1}{\beta} (p(t) - p(t_n)) &= \int_{t_n}^t \exp \left[-\beta \int_s^t \gamma(q(u)) du \right] \left(\bar{K}(y(s)) ds + \bar{\delta}(y(s)) dW_s \right) \\ &\quad + \frac{1}{\beta} p(t_n) \left\{ \exp \left[-\beta \int_{t_n}^t \gamma(q(s)) ds \right] - 1 \right\} \end{aligned} \tag{5.11}$$

An easy computation using (4.6) shows that $\hat{y}(t) = \Gamma(\hat{q}(t))$ is given by

$$\hat{y}(t) - \hat{y}(t_n) = \int_{t_n}^t \bar{K}(\hat{y}(s)) ds + \int_{t_n}^t \bar{\delta}(\hat{y}(s)) dW_s \tag{5.12}$$

By virtue of (5.2)

$$\begin{aligned} \lim_{\beta \rightarrow \infty} E(|q(t) - \hat{q}(t)|^2) &= \lim_{\beta \rightarrow \infty} E(|\Gamma^{-1}(y(t)) - \Gamma^{-1}(\hat{y}(t))|) \\ &\leq A^2 \lim_{\beta \rightarrow \infty} E(|y(t) - \hat{y}(t)|^2) \end{aligned}$$

and thus (5.7) follows, if we show that for $t \in [0, \infty)$

$$\lim_{\beta \rightarrow \infty} E(|y(t) - \hat{y}(t)|^2) = 0 \tag{5.13}$$

To show (5.13) we take the difference of (5.10) and (5.12) and inserting (5.11) we obtain, after standard adding and subtracting procedure:

$$\begin{aligned} |\hat{y}(t) - y(t)| &\leq |\hat{y}(t_n) - y(t_n)| + \int_{t_n}^t |\bar{K}(\hat{y}(s)) - \bar{K}(y(s))| ds \\ &\quad + \left| \int_{t_n}^t [\bar{\delta}(\hat{y}(s)) - \bar{\delta}(y(s))] dW_s \right| \\ &\quad + \int_{t_n}^t \exp \left[-\beta \int_s^t \gamma(q(u)) du \right] |\bar{K}(y(s)) - \bar{K}(\hat{y}(s))| ds \\ &\quad + \left| \int_{t_n}^t \exp \left[-\beta \int_s^t \gamma(q(u)) du \right] [\bar{\delta}(\hat{y}(s)) - \bar{\delta}(y(s))] dW_s \right| \\ &\quad + \int_{t_n}^t \exp \left[-\beta \int_s^t \gamma(q(u)) du \right] |\bar{K}(\hat{y}(s))| ds \\ &\quad + \left| \int_{t_n}^t \exp \left[-\beta \int_s^t \gamma(q(u)) du \right] \bar{\delta}(\hat{y}(s)) dW_s \right| + \frac{1}{\beta} |p(t_n)| \end{aligned}$$

Next we use the fact that for Itô integrals for nonanticipating functions $g(s)$:

$$E\left(\left|\int_0^t g(s) dW_s\right|^2\right) = \int_0^t E(|g(s)|^2) ds$$

and taking the expectation of the square we get

$$\begin{aligned} & E(|\hat{y}(t) - y(t)|^2) \\ & \leq 8E(|\hat{y}(t_n) - y(t_n)|^2) + 8(t - t_n) \int_{t_n}^t E(|\bar{K}(\hat{y}(s)) - \bar{K}(y(s))|^2) ds \\ & \quad + 8 \int_{t_n}^t E(|\bar{\delta}(\hat{y}(s)) - \bar{\delta}(y(s))|^2) ds + 8(t - t_n) \\ & \quad \times \int_{t_n}^t E\left(\exp\left[-2\beta \int_s^t \gamma(q(u)) du\right] |\bar{K}(\hat{y}(s)) - \bar{K}(y(s))|^2\right) ds \\ & \quad + 8 \int_{t_n}^t E\left(\exp\left[-2\beta \int_s^t \gamma(q(u)) du\right] |\bar{\delta}(\hat{y}(s)) - \bar{\delta}(y(s))|^2\right) ds \\ & \quad + 8(t - t_n) \int_{t_n}^t E\left(\exp\left[-2\beta \int_s^t \gamma(q(u)) du\right] \bar{K}^2(\hat{y}(s))\right) ds \\ & \quad + 8 \int_{t_n}^t E\left(\exp\left[-2\beta \int_s^t \gamma(q(u)) du\right] \bar{\delta}^2(\hat{y}(s))\right) ds + \frac{8}{\beta^2} E(p(t_n)^2) \end{aligned}$$

For this we have used two inequalities:

- (i) $\left(\sum_{i=1}^N a_i\right)^2 \leq N \sum_{i=1}^N a_i^2$
- (ii) Schwartz inequality: $\left(\int_{t_n}^t h(s) ds\right)^2 \leq (t - t_n) \int_{t_n}^t h^2(s) ds$

We now employ (5.3), (5.4), and $\gamma \geq a > 0$ and introduce

$$\varphi(t) = E(|\hat{y}(t) - y(t)|^2)$$

to obtain

$$\begin{aligned} \varphi(t) &\leq 8\varphi(t_n) + 16(t - t_n)^2 B^2 \sup_{t \in \Delta_n} \varphi(t) + 16(t - t_n) C^2 \sup_{t \in \Delta_n} \varphi(t) \\ &\quad + 8(t - t_n) \int_{t_n}^t e^{-2\beta a(t-s)} E(\bar{K}^2(\hat{y}(s))) ds \\ &\quad + 8 \int_{t_n}^t e^{-2\beta a(t-s)} E(\bar{\delta}^2(\hat{y}(s))) ds + \frac{8}{\beta^2} E(p(t_n)^2) \end{aligned}$$

This is true for all $t \in \Delta_n$, hence we can replace the left-hand side by $\sup_{t \in \Delta_n} \varphi(t)$ and in view of (5.9) we end up with

$$\begin{aligned} \sup_{t \in \Delta_n} \varphi(t) &\leq 16\varphi(t_n) + 16|\Delta_n| \int_{t_n}^t e^{-2\beta a(t-s)} E(\bar{K}^2(\hat{y}(s))) ds \\ &\quad + 16 \int_{t_n}^t e^{-2\beta a(t-s)} E(\bar{\delta}(\hat{y}(s))^2) ds + \frac{16}{\beta^2} E(p(t_n)^2) \quad (5.14) \end{aligned}$$

It is easy to see that the integrals on the right-hand side of (5.14) go to zero as $\beta \rightarrow \infty$ if $E(\bar{K}^2(\hat{y}(s)))$ and $E(\bar{\delta}^2(\hat{y}(s)))$ are continuous functions of s . But $E(p(t_n)^2) \leq 2E(|p(t_n) - p_0|^2) + 2p_0^2$. Use (5.11) for $t = t_n$ and $t_n = 0$ to obtain $1/\beta(p(t_n) - p_0)$ and proceed analogously as above to get with some constant D

$$\lim_{\beta \rightarrow \infty} \frac{32}{\beta^2} E(|p(t_n) - p_0|^2) \leq D \lim_{\beta \rightarrow \infty} \sup_{0 < t \leq t_n} \varphi(t)$$

We are left with

$$\lim_{\beta \rightarrow \infty} \sup_{t \in \Delta_n} \varphi(t) \leq 16 \lim_{\beta \rightarrow \infty} \varphi(t_n) + D \lim_{\beta \rightarrow \infty} \sup_{0 < t \leq t_n} \varphi(t)$$

At $t_0 = 0$, $\hat{y}(0) = \Gamma(\hat{q}(0)) = \Gamma(q(0)) = y(0) = y_0$, i.e.,

$$\varphi(t_0) = E(|\hat{y}(0) - y(0)|^2) = 0$$

and so

$$\lim_{\beta \rightarrow \infty} \sup_{t \in \Delta_0} \varphi(t) = 0$$

where $\Delta_0 = [0, t_1]$, $t_1 > 0$. Equation (5.13) follows now by induction over n . ■

Remark. The weak convergence of the Smoluchowski limit follows as a special case from general theorems established in Ref. 22 as pointed out by H. Spohn to one of the authors (D.D.).

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