The overdamped limit for the Brownian motion in an inhomogeneous medium

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We revisit the problem of the overdamped limit of the Brownian dynamics in an inhomogeneous medium characterized by a position-dependent friction coefficient and a multiplicative noise in one space dimension. Starting from the Kramers equation and analyzing it through the expansion in terms of the eigenfunctions of the quantum harmonic oscillator, we derive analytically the corresponding Fokker-Planck equation in the large friction (overdamped) limit. The result is fully consistent with the previous finding by Sancho, San Miguel, and Dürr [2], but our derivation procedure is simple and transparent. Furthermore, it would be straightforward to obtain higher-order corrections systematically. We also show that the overdamped limit is equivalent to the mass-zero limit in general. Our results are confirmed by numerical simulations for simple examples.

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The stochastic differential equation (SDE) with a multiplicative noise always brings a basic question about what is the correct choice in representing the noise integration, so called the noise calculus with various types: Ito, Stratonovich, anti-Ito, and others. One consensus is that the noise calculus itself is a part of the problem that should be provided experimentally or theoretically prior to inferring the SDE [1].

The Brownian motion of a colloidal particle suspended in a spatially inhomogeneous medium is such an example. The medium inhomogeneity can be characterized, in general, by space dependence of the friction coefficient and the local temperature (or the diffusion coefficient). The naive Langevin description in the overdamped (large friction) limit led to the SDE with a multiplicative noise, which raised a question of the noise calculus choice, the so-called Ito-Stratonovich dilemma. However, it is clear that the corresponding underdamped Langevin equation does not depend on the noise calculus, thus the overdamped limit should not depend on it, either.

This dilemma was settled down thirty years ago by Sancho, San Miguel, and Dürr (SSMD) [2] for most general cases. They successfully integrated out the fast variable (velocity) of the underdamped Langevin equation in the large friction limit by the so-called adiabatic elimination procedure, an extended version of the work done by Haken [3]. Interestingly, their results do not correspond to any choice of the noise calculus in the naive Langevin description, in general, except a couple of cases. However, this derivation is quite involved and mixes up the Langevin equation approach with the Fokker-Planck type description. And their results have never been tested against numerical simulations. These might cause some confusions, which triggered several recent works on this already resolved Ito-Stratonovich dilemma [4,5].

For a simpler case with a constant friction coefficient (still space-dependent local temperature), the overdamped limit was rigorously derived by the Fokker-Planck equation approach [6] and also by the Langevin equation approach at the level of a single realization [10]. This case turns out to correspond to the naive Langevin description with the Ito calculus. The other simpler case with a constant temperature with a space-dependent friction coefficient was also studied and the Fokker-Planck equation in the overdamped limit was rigorously derived [5,11], which is equivalent to the naive Langevin description with the anti-Ito calculus. However, the same type of derivation was not possible for more general cases, prior to our present work. It should be noted that, very recently, Yang and Ripoll [5] succeeded to yield the correct overdamped limit for general cases (consistent with the SSMD result), through the Langevin equation approach by assuming the macroscopic force balance condition for the averaged quantities.

In this study, we derive the correct overdamped limit rigorously and transparently by the Fokker-Planck approach for general cases without any assumption. We start with the Kramers equation for the underdamped Langevin equation, which is independent of the noise calculus. With some operator transformations, we obtain the time-dependent probability distribution function in terms of the eigenfunctions of the quantum harmonic oscillator, similar to the method employed by Risken [11]. This approach allows for a systematic expansion of the Kramers equation in the large friction limit. Keeping up to the first order, we find the same overdamped Fokker-Planck equation as in the SSMD. We present the numerical simulation results for simple examples, which are in excellent accord with our analytic results. Finally, we show that the overdamped limit is generally equivalent to the mass zero limit which was previously known only when the Einstein relation (constant temperature) holds [5].

We consider the underdamped Langevin equation for the one-dimensional Brownian motion of a colloidal particle in an inhomogeneous medium, which is described by the second order SDE as

\[ m\ddot{x} = -\gamma(x)\dot{x} + f(x) + g(x)\xi(t), \]  

where \( \gamma(x) \) is the friction coefficient and \( g(x) \) the noise.
strength, both of which depend on position \( x \). \( \xi(t) \) is a white noise satisfying \( \langle \xi(t)\xi(t') \rangle = 2\delta(t-t') \). Even though the noise is multiplicative (position-dependent), the choice of the noise calculus is meaningless because the stochastic noise \( g(x)\xi(t) \) directly affects the velocity variation rather than the position variation in the second order SDE. This will be clear in the probability description, i.e. Kramers equation later.

The naive approach to the overdamped limit begins with neglecting the inertia term in the left hand side of the equation, because the overdamped limit is defined in the regime of \( \gamma \gg (\Delta t)^{-1} \) with coarse-graining time scale \( \Delta t \). Then, we may end up with

\[
\dot{x} = \frac{f(x)}{\gamma(x)} + \frac{g(x)}{\gamma(x)} \xi(t).
\]

However, this equation depends on the noise calculus because the stochastic noise here directly changes the position instantly, so it will be crucial when the noise strength \( g(x)/\gamma(x) \) should be evaluated during the integration of the equation over time interval \( \Delta t \). This dependence of the noise calculus causes the Ito-Stratonovich dilemma. Therefore, the above naive overdamped Langevin equation cannot be a correct one to describe the overdamped limit of the noise-calculus-independent underdamped equation. For its correct description, one should carefully take the proper large \( \gamma \) limit, in particular, for the noise-induced drift force and then integrate out the velocity (fast) degree of freedom in the underdamped equation.

For later convenience, we first discuss the noise-calculus dependence of Eq. (2). By integrating it during the time interval \([t, t + \Delta t]\), one can get the equation for \( \Delta x \equiv x(t + \Delta t) - x(t) \) as

\[
\Delta x = \left( \frac{f}{\gamma} + \frac{2\alpha g}{\gamma} \right) \Delta t + \left( \frac{g}{\gamma} \right) \Delta W,
\]

where \( \Delta W = \int_0^{\Delta t} ds \xi(s) \) is called the Wiener process, satisfying \( \langle \Delta W \rangle = 0, \langle (\Delta W)^2 \rangle = 2\Delta t \). The noise calculus parameter \( \alpha \in [0,1] \) specifies when the noise amplitude function \( h = g/\gamma \) is evaluated, such that \( \int_0^{\Delta t} ds h(x(s)) \xi(s) \) is replaced by \( h(x^*) \Delta W \) with an intermediate value \( x^* = (1 - \alpha)x(t) + \alpha x(t + \Delta t) \). Various noise calculi depend on \( \alpha \): the Ito (\( \alpha = 0 \)), the Stratonovich (\( \alpha = 1/2 \)), the anti-Ito or isothermal (\( \alpha = 1 \)). Employing the Taylor expansion of the noise amplitude function \( h(x^*) \) and the subsequent iteration procedure, the stochastic term can be decomposed into last two terms as above. The subscript I (Ito) in the last term indicates that the noise amplitude function should be evaluated at the initial time \( t \) for the Wiener process. The second term is the additional drift force induced by the noise calculus where the superscript ' represents the derivative as \( h' = \partial h/\partial x \). Note that this term vanishes when the noise amplitude function \( h(x) \) is independent of position \( x \).

Following the standard procedure involving the Kramers-Moyal coefficients [1,11], it is easy to derive the corresponding Fokker-Plank equation for the probability distribution function \( P(x,t) \) as

\[
\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ -\frac{f}{\gamma} - \alpha \frac{T}{\gamma} + \frac{\partial}{\partial x} T \right] P(x,t)
\]

where the local temperature \( T(x) \) is defined by \( T(x) \equiv g^2(x)/\gamma(x) \), called as the generalized Einstein relation.

Now, we return to the underdamped Langevin equation, Eq. (4). It is well known that the corresponding probability evolution (Kramers) equation can be written as

\[
\partial_t P(x,v,t) = (L_{\text{rev}} + L_{\text{irr}}) P(x,v,t)
\]

with

\[
L_{\text{rev}} = -v \partial_x - (f/m) \partial_v , \quad L_{\text{irr}} = (\gamma/m) \partial_v [v + (T/m) \partial_v],
\]

where \( \partial_y \equiv \partial/\partial y \) (\( y = t, v, x \)). The reversible operator \( L_{\text{rev}} \) describes the deterministic motion, while the irreversible operator \( L_{\text{irr}} \) describes the thermal stochastic motion. As discussed before, there is no dependence of the noise calculus in the Kramers equation, in contrast to Eq. (4).

From now on, we set \( m = 1 \) for simplicity. It is convenient to put \( L_{\text{irr}} \) into a Hermitian form via a similarity transformation, using the stationary solution of \( L_{\text{irr}} \), as \( P_{\text{irr}}^* (v,T) = (2\pi T)^{-1/2} e^{-v^2/2T} \) [11]. Then, the Hermitianized operator \( \bar{L}_{\text{irr}} \) is given as

\[
\bar{L}_{\text{irr}} = [P_{\text{irr}}^*]^{-1/2} L_{\text{irr}} [P_{\text{irr}}^*]^{1/2} = \gamma \left( T \partial_v^2 - \frac{v^2}{4T} + \frac{1}{2} \right)
\]

which is identical to the Hamiltonian operator of the quantum harmonic oscillator. Introducing the lowering and raising ladder operators \( b \) and \( b^\dagger \), we get

\[
\bar{L}_{\text{irr}} = -\gamma b^\dagger b
\]

with

\[
b = \sqrt{T} \partial_v + \frac{v}{2\sqrt{T}}, \quad b^\dagger = -\sqrt{T} \partial_v + \frac{v}{2\sqrt{T}}
\]

Then, the orthonormal eigenfunctions of \( \bar{L}_{\text{irr}} \) are given by

\[
\psi_n(v,T) = (2\pi T)^{-1/4} \exp \left[ -v^2/(4T) \right] = [P_{\text{irr}}^*]^{1/2} \psi_n(v,T) = b^\dagger \psi_{n-1}(v,T)/\sqrt{2n}
\]

\[
= \psi_0(v,T) H_n(v\sqrt{2T})/\sqrt{n!2^n}
\]

where \( H_n \) are the Hermite polynomials (\( n = 1,2,\ldots \)). Note that these eigenfunctions depend on position \( x \) through \( T(x) \). For the operator \( L_{\text{rev}} \), the same procedure gives

\[
\bar{L}_{\text{rev}} = \psi_0(v,T)^{-1} (-v \partial_x - f \partial_v) \psi_0(v,T)
\]

\[
= -\psi_0^\dagger \partial_v \sqrt{T} \psi_0 (b + b^\dagger) + \frac{f}{\sqrt{T}} b^\dagger
\]
With these transformed operators, Eq. (5) obviously becomes
\[ \partial_t \bar{P}(x, v, t) = (\bar{L}_{\text{rev}} + \bar{L}_{\text{irr}}) \bar{P}(x, v, t) \] (12)
with \( \bar{P}(x, v, t) = \psi_0^{-1} P(x, v, t) \). Therefore, one can perform an expansion in terms of \( \{ \psi_n \} \)
\[ \bar{P}(x, v, t) = \sum_{n=0}^{\infty} c_n(x, t) \psi_n(v, T) \] (13)
The transformed operators act on \( \bar{P} \) in the following way
\[ \bar{L}_{\text{irr}} \bar{P} = -\gamma \sum_{n=0}^{\infty} n c_n(x, t) \psi_n(x, T) \] (14)
\[ \bar{L}_{\text{rev}} \bar{P} = -\sum_{n=0}^{\infty} \left( [Dc_n] b \psi_n + [Dc_n] b^\dagger \psi_n \right. \\
+ c_n \psi_0^{-1} \partial_x \sqrt{T} \psi_0(b + b^\dagger) \psi_n \right) \]
where \( D = \sqrt{T} \partial_x, \hat{D} = \sqrt{T} \partial_x - f/\sqrt{T} \) and the \([ \cdots ] \) means that the operator acts only inside. When \( T \) is a constant, \( \{ \psi_n \} \) is independent of \( x \) and the last term of \( \bar{L}_{\text{rev}} \bar{P} \) drops out, which simplifies the algebra.

For general \( T(x) \), a straightforward algebra yields with the help of the Hermite polynomial recurrence relation property, \( H'_n/H_n = \sqrt{2n} \psi_{n-1}/\psi_n \), that
\[ \partial_t \bar{P} = -\sum_{n=0}^{\infty} \left( \gamma n c_n + [Dc_n] b + [Dc_n] b^\dagger \right. \\
+ \left. \left( \sqrt{T} \right)' c_n (b + b^\dagger) b^{\dagger} (b + b^\dagger) \right) \psi_n . \] (15)
From this equation, one can easily extract the hierarchy of the expansion coefficients \( c_n(x, t) \) as
\[ \partial_t c_n = -\gamma n c_n - (n + 1)^{1/2} D c_{n+1} - n^{1/2} \hat{D} c_{n-1} \\
- \left( \sqrt{T} \right)' c_n + 2n^{-3/2} c_{n+1} + 2n^{3/2} c_{n-1} \\
+ \sqrt{n(n-1)(n-2)} c_{n-3} \ , \] (16)
which is a generalized version of the so-called Brinkman’s hierarchy \([11, 12]\). We emphasize that all results are rigorous without any approximation up to now.

Now, we take the overdamped limit of \( \gamma \gg (\Delta t)^{-1} \), in such a way that \( \partial_t c_n \) is neglected in comparison with \( \gamma c_n \) for \( n \geq 1 \) in Eq. (16). Considering the remaining terms in the order of the power of \( \gamma^{-1} \), one can easily show that \( c_n \sim O(\gamma^{-n}) \) for \( n = 0, 1, 2 \) and \( c_n \sim O(\gamma^{-(n-2)}) \) for \( n \geq 3 \). Note that the last term proportional to \( c_{n-3} \) in Eq. (16) makes \( c_n \) behave distinctly for \( n \leq 2 \) and \( n \geq 3 \). Up to \( O(\gamma^{-1}) \), there remain only three equations as
\[ 0 = \partial_t c_0 + \left[ D + \left( \sqrt{T} \right)' \right] c_1, \]
\[ 0 = \gamma c_1 + \left[ \hat{D} + 2 \left( \sqrt{T} \right)' \right] c_0, \]
\[ 0 = 3\gamma c_3 + \sqrt{6} \left( \sqrt{T} \right)' c_0 . \] (17)
By combining the first two equations, we get the partial differential equation for \( c_0(x, t) \) as
\[ \partial_t c_0 = \left[ D + \left( \sqrt{T} \right)' \right] \gamma^{-1} \left[ \hat{D} + 2 \left( \sqrt{T} \right)' \right] c_0 \]
\[ = \partial_x \left[ -f + \frac{1}{\gamma} \partial_x T \right] c_0 . \] (18)
By solving this equation for \( c_0 \), and rewriting \( c_1 \) and \( c_3 \) in terms of \( c_0 \) as given in Eq. (17), we finally get the solution for \( \bar{P}(x, v, t) = \psi_0 P(x, v, t) \) through Eq. (13) for the large \( \gamma \) limit.

In this work, we are interested in the probability distribution function of position \( x \), integrated over velocity \( v \) as
\[ \bar{P}(x, t) = \int_{-\infty}^{+\infty} dv \ P(x, v, t) \]
\[ = \int_{-\infty}^{+\infty} dv \psi_0(v, T) \bar{P}(x, v, t) = c_0(x, t) \]
where the orthonormal property of \( \{ \psi_n \} \) is used. Thus, we find
\[ \partial_t \bar{P}(x, t) = \partial_x \left[ -f + \frac{1}{\gamma} \partial_x T \right] \bar{P}(x, t) \] (20)
This result is exactly the same as the SSMD result, Eq. (2.18) in \([2]\), so our rigorous and transparent derivation confirmed the SSMD result \([13]\).

It is certainly different from the naive result in Eq. (4). First, it is independent of the noise calculus, \( \alpha \). Moreover, any choice of \( \alpha \) in Eq. (4) cannot generate our result in general. The naive result with the anti-Ito choice \( (\alpha = 1) \) happens to be identical to our result, only when \( T \) is a constant \([1, 5, 11]\). The Ito calculus \( (\alpha = 0) \) also happens to give a correct result, only when \( \gamma \) is a constant \([5, 11]\).

The correct and general Langevin equation corresponding to the above Fokker Plank equation, Eq. (20), can be written as
\[ \dot{x} = f + T \left( \frac{1}{\gamma} \right)' - \alpha \left( \frac{T}{\gamma} \right)' + \sqrt{\frac{T}{\gamma}} \xi(t) , \] (21)
where the noise-calculus-dependent drift force is included to cancel out the additional drift term induced by the multiplicative noise. This inclusion implies that the naive approach with an extra physical drift force cannot describe the correct overdamped limit in general.

We will confirm our result Eq. (20) by numerical simulations for simple examples. First, we perform numerical integrations of the second order SDE, Eq. (4), for a large \( \gamma \). Casting the second order SDE into a set of two first order SDEs and integrating them during the time interval \([t, t + \Delta t] \), we get
\[ \Delta x = v \Delta t , \]
\[ \Delta v = (-\gamma v + f) \Delta t + (\sqrt{\gamma}) \Delta W , \] (22)
Finally we compare the results from Eq. (22) with those obtained from Eq. (23) and Eq. (24), respectively, which overlap each other very well. Squares (Ito) and triangles (anti-Ito) represent the data obtained from Eq. (24) with \( \alpha = 0 \), 1, respectively.

where we set \( m = 1 \) and choose the Ito calculus for convenience without loss of generality for small \( \Delta t \). Here, we take \( \Delta t = 10^{-3} \) and the initial distributions are gaussian with variance 2 centered on \( x = 1 \) for the position and centered on \( v = 0 \) for the velocity. To obtain a reasonable accuracy for the probability distribution function, we repeat simulations for \( 2 \sim 5 \times 10^6 \) samples.

Next we perform numerical simulations, using our result of Eq. (21) with \( \alpha = 0 \) (identical with any other choice of \( \alpha \)) as

\[
\Delta x = \left[ \frac{f}{\gamma} + T \left( \frac{1}{\gamma} \right) \right] \Delta t + \left( \frac{T}{\gamma} \right) I \Delta W ,
\]

and also using the naive result of Eq. (13)

\[
\Delta x = \left[ \frac{f}{\gamma} + \alpha \left( \frac{T}{\gamma} \right) \right] \Delta t + \left( \frac{T}{\gamma} \right) I \Delta W .
\]

Finally we compare the results from Eq. (22) with those from Eq. (23) and Eq. (24).

In the first example, we take \( \gamma(x) = c(1 + e^{-x^2/2}) \) and \( T(x) = 2/(1 + e^{-x^2/2})(1 + 2x^2)^2 \) with \( f(x) = 0 \). In Fig. 1 one can easily see that the naive overdamped limit with either \( \alpha = 1 \) or \( \alpha = 0 \) does not fit to the data points obtained from Eq. (22), though the latter seems to fit better by chance. However, our overdamped limit given by Eq. (23) gives an excellent agreement. In the second example, we take \( \gamma(x) = c(\frac{3}{2} + \frac{2x}{\sqrt{x^2 + 1}}) \) and \( T(x) = (3 + \frac{4x}{\sqrt{x^2 + 1}})^2/[4(3 + \frac{4x}{\sqrt{x^2 + 1}})] \) with \( f(x) = -2x \). Again, the data in Fig. 2 show us the perfect agreement between our overdamped limit given by Eq. (23) and the stochastic differential equation of Eq. (24).

Finally, we discuss the mass zero limit of Eq. (1). Ao et al. derived the Fokker Planck equation in the mass zero limit when \( T = constant \). Here, we extend their result to the general case where \( T = T(x) \). Starting from the Kramers equation given by Eqs. (5) and (6), we change the variables such that \( s = t/\sqrt{m} \) and \( u = v\sqrt{m} \) to obtain the covariant form of the Kramers equation in terms of variables \( (x, u, s) \) as

\[
\partial_s P(x, u, s) = \left( L_{rev} + L_{irr} \right) P(x, u, s)
\]

with

\[
L_{rev} = -u\partial_x - f\partial_u , \quad L_{irr} = \gamma_m \partial_u \left[ u + T \partial_u \right] ,
\]

with \( \gamma_m = \gamma/\sqrt{m} \). These equations are the same as Eqs. (5) and (6) by replacing \( \gamma \) by \( \gamma_m \) and setting \( m = 1 \).

It is obvious that the mass zero limit \( (m \rightarrow 0) \) is equivalent to the large \( \gamma_m \) limit as long as \( \gamma \) does not vanish. Thus, one can perform exactly the same transformation as we did with the variable \( \gamma_m \) and take the large \( \gamma_m \) limit to obtain

\[
\partial_s \hat{P}(x, s) = \partial_x \left[ -\frac{f}{\gamma_m} + \frac{1}{\gamma_m} \partial_x T \right] \hat{P}(x, s) .
\]

By returning back to the original variables of \( (x, t) \), we can easily recover Eq. (20). This proves that the mass zero limit is equivalent to the overdamped limit for general cases. We check this result by numerical simulations when \( T \) is not a constant with \( \gamma(x) = 1 + e^{-x^2/2}, T(x) = 1/[2(1 + e^{-x^2/2})(x^2 + 1)^2], \) with \( f(x) = -x/5 \). Again we have an excellent agreement between the simulations on the original second order SDE and our equation in the mass zero limit.

To summarize, we derive the correct overdamped Fokker Planck equation for the Brownian motion in a general inhomogeneous medium with a position-dependent friction coefficient as well as a position-dependent temperature. Our result is consistent with
We take \( \gamma(x) = 1 + e^{-x^2/2} \), \( T(x) = 1/[2(1 + e^{-x^2/2})(x^2 + 1)^2] \), and \( f(x) = -x/5 \) with a small value of \( m = 0.01 \). The same symbols are used as in Fig. 1.

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