Derivation of the Langevin equation from the principle of detailed balance

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Abstract. For a system at a given temperature, with the energy known as a function of a set of variables, we obtain the thermal fluctuation of the evolution of the variables by replacing the phase space with a lattice and invoking the principle of detailed balance. The asset of this method, besides its simplicity, is that it enables us to obtain the Langevin equation when the phase space is anisotropic and when the system is described by means of curvilinear coordinates. As an illustration, we apply our results to the Kramer–Watts-Tobin equation in superconductivity. The choice between the Itô and the Stratonovich procedures is discussed.

Keywords: molecular dynamics
1. Introduction

In this paper we deal with what we call ‘purely diffusive systems’ in contact with a thermal bath. By this we mean systems with a state described by microscopic variables $x_1, \ldots, x_N$, with energy $E(x_1, \ldots, x_N)$, which in the absence of thermal fluctuations are expected to follow an evolution equation

$$ \frac{dx_j}{dt} = -\Gamma_j(x_1, \ldots, x_N) \frac{\partial E}{\partial x_j}, $$

(1)

where $t$ is the time and the positive coefficients $\Gamma_j$ are determined by the dynamics of the system and its interaction with its environment. $\partial E/\partial x_j$ may be regarded as a driving force and $\Gamma_j$ as a compliance coefficient. The Langevin approach tells us that the influence of thermal fluctuations can be taken into account by adding a fluctuating quantity in the right-hand side of the evolution equation; this fluctuating quantity is called the ‘Langevin term’.

The paradigm of a purely diffusive system is a particle that undergoes Brownian motion. In this case the variable is its momentum, $E$ is its kinetic energy and $\Gamma$ is the Stokes coefficient. Paul Langevin dealt with this problem [1] and determined the variance of the Langevin term by invoking the theorem of the equipartition of the kinetic energy among the various degrees of freedom of a system in thermal equilibrium. Gillespie [2] notes that it is not obvious that the influence of fluctuations can be separated as an additive term with zero average; regarding the velocity evolution as a Markovian process and assuming that the ‘stepping functions’ (which will be defined in section 2) are linear functions of velocity, it is shown that this separation does indeed occur. Katayama and Terauti [3] used the Langevin equation to study the Brownian motion of a single particle...
under steady plane shear flow. Balescu [4] introduces a Langevin equation in a model for the description of a plasma. Bringuier [5] discusses the difficulties encountered when applying the Langevin approach to the Hall effect. The relation between the Langevin and the Klein–Kramers approaches is discussed in [6].

During the century that has elapsed since Langevin’s paper, his approach has been extended to wide classes of problems in Physics [7]–[10] and the Langevin term is determined by means of the fluctuation-dissipation theorem [11]–[13]. In this paper we will evaluate the distribution of the Langevin term by means of the principle of detailed balance [12].

The tools for handling the problems considered in this paper may be found in the literature on stochastic differential equations (e.g. [14]–[16]) and many of the questions raised here may be avoided by switching to the Fokker–Planck equation; this paper is addressed to those readers, presumably physicists, who prefer a more intuitive approach.

2. Our method

2.1. The 1D case

We consider a one-dimensional system with microscopic state determined by the variable \( x \). We discretize \( x \) and assume that its possible values are \( x_i = i\ell \), where \( \ell \) is a ‘lattice constant’. We denote by \( \epsilon_i = E(x_{i+1}) - E(x_i) \) the energy difference between consecutive lattice points. We assume now that for a short period of time \( \delta t \) the probability of passing from \( x_i \) to \( x_{i \pm 1} \) is given by \( W_{i \pm \delta t} \), where \( W_{i+} \) and \( W_{i-} \) are ‘stepping functions’ that stand for the transition probability rates.

The principle of detailed balance asserts that in thermal equilibrium the probability for a transition from \( i \) to \( i + 1 \) equals that for a transition in the opposite direction, i.e.,

\[
P_{i \rightarrow i+1} = P_{i+1 \rightarrow i}.
\]

Since \( P_{i \rightarrow i+1} = e^{\epsilon_i/kT} \), where \( k_B \) is the Boltzmann constant and \( T \) is the temperature,

\[
W_{i+1,-} = W_{i,+} e^{\epsilon_i/kT}.
\] (2)

It should be noted that not every system obeys detailed balance. Denoting by \( P_i \) the probability for \( x = x_i \) (not necessarily for equilibrium), \( P_i W_{i,+} - P_{i+1} W_{i+1,-} \) stands for the probability current. Detailed balance requires that this current vanishes, whereas in order to maintain a stationary state it is sufficient that the divergence of the current vanishes. If probability currents are present in equilibrium, it follows that there are driving forces which cannot be expressed as the gradient of the energy as in equation (1) (such as the magnetic force on a charged particle). Therefore, systems that do not obey detailed balance are beyond the scope of this paper.

In order to obtain more symmetric expressions, we write \( W_{i,+} = w_i \lambda_i \), \( W_{i,-} = w_i / \lambda_i \) and, taking \( \ell \) sufficiently small that quantities of order \( O(\ell^2) \) can be dropped, we write \( w_{i \pm 1} = w_i \pm w_i' \) and \( \lambda_{i \pm 1} = \lambda_i \pm \lambda_i' \), where \( w_i' / w_i \) and \( \lambda_i' \) are at most of order \( O(\ell) \). With this notation and approximation, equation (2) becomes

\[
\frac{w_i + w_i'}{\lambda_i + \lambda_i'} = w_i \lambda_i e^{\epsilon_i/kT}.
\] (3)
Similarly, requiring detailed balance between the sites $i$ and $i-1$ we obtain
\begin{equation}
(w_i - w'_i)(\lambda_i - \lambda'_i)e^{\epsilon_i/k_B T} = \frac{w_i}{\lambda_i},
\end{equation}
where we have exchanged sides in the equation and neglected the $O(\ell^2)$ difference $\epsilon_{i-1} - \epsilon_i$. Multiplying the equations (3) and (4) and neglecting the $O(\ell^2)$ term $(w'_i/w_i)^2$ we obtain
\begin{equation}
\frac{\lambda_i - \lambda'_i}{\lambda_i + \lambda'_i} = 1,
\end{equation}
and hence $\lambda'_i$ is of order $O(\ell^2)$ and will be dropped. $\lambda_i$ can now be obtained from equation (3); keeping terms of order $O(\ell)$ and making use of the definitions of $w'_i$ and $\epsilon_i$, it becomes
\begin{equation}
\lambda_i = \sqrt{(1 + w'_i/w_i)e^{-\epsilon_i/k_B T}} = 1 + w'_i/(2w_i) - \epsilon_i/(2k_B T) \\
= 1 + (\ell/2) d[\log(w)]/dx - [\ell/(2k_B T)]dE/dx,
\end{equation}
where we have defined a smooth function $w$ such that $w(x_i) = w_i$.

Let us denote by $\delta x$ the increment of the variable $x$ during the period of time $\delta t$. For sufficiently small $\delta t$ we can neglect multiple transitions and the possible values of $\delta x$ are 0 and $\pm \ell$. The average value of $\delta x$ will be
\begin{equation}
\langle \delta x \rangle = \ell w_i \delta t(\lambda_i - 1/\lambda_i) = \ell^2 w \delta t[\log(w)]/dx - (1/(k_B T))dE/dx,
\end{equation}
where in the last step we have neglected higher orders of $\ell$ and have dropped the index $i$.

Similarly, the variance of $\delta x$ will be
\begin{equation}
\langle (\delta x)^2 \rangle = \ell^2 w \delta t(\lambda_i + 1/\lambda_i) = 2\ell^2 w \delta t,
\end{equation}
where besides dropping terms that are of higher order in $\ell$ we have used the fact that, for small $\delta t$, $\langle (\delta x)^2 \rangle \ll \langle (\delta x)^2 \rangle$.

We now get rid of the unphysical lattice by defining $\Gamma(x) = \ell^2 w(x)/(k_B T)$. With this notation equations (7) and (8) become
\begin{equation}
\langle \delta x \rangle = \Gamma(x) \delta t[k_B T d[\log(\Gamma)]/dx - dE/dx],
\end{equation}
and
\begin{equation}
\langle (\delta x)^2 \rangle = 2k_B T \Gamma(x) \delta t.
\end{equation}
Finally, we consider a lapse of time $\tau$ which is very short compared with the relaxation time, but very long compared with $\delta t$. By the central limit theorem [12, 17, 18], the increment of $x$ (which is the sum of many increments described by equation (9)) will be
\begin{equation}
\Delta x = \Gamma(x) [k_B T d[\log(\Gamma)]/dx - dE/dx] \tau + \eta,
\end{equation}
where $\eta$ is a fluctuating term with average 0, variance $2k_B T \Gamma(x) \tau$ and Gaussian distribution. $\eta$ is the Langevin distribution that we were looking for. There is still a subtle question concerning the precise value of $x$ at which $\Gamma(x)$ has to be evaluated; this issue is considered in appendix A.

Let us now compare the nonfluctuating part of equation (11) with equation (1). If $\Gamma$ is independent of $x$, equation (1) is recovered; otherwise, there is also a drift term $k_B T d[\log(\Gamma)]/dx$ that pushes $x$ towards values where $\Gamma$ is larger. The drift term can be absorbed into equation (1) if we replace the energy $E$ by $G = E - k_B T \log(\Gamma)$.

The term $k_B T \log(\Gamma)$ may be regarded as a sort of chemical potential, where $\Gamma$ plays the role of the activity.

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2.2. The multivariable system

We consider now a system with variables \( x_1, \ldots, x_N \). For each of the variables we can repeat the analysis of the previous section and equation (11) generalizes to

\[
\Delta x_j = -\Gamma_j(\partial G_j/\partial x_j)\tau + \eta_j,
\]

(12)

with \( G_j = E - k_B T \log \Gamma_j \) and \( \eta_j \) is a Langevin function with average 0, variance \( 2k_B T \Gamma_j \tau \) and Gaussian distribution.

We might also be interested in the evolution of other variables rather than those in the set \( x_1, \ldots, x_N \). This problem is considered in appendix B.

2.3. Curvilinear coordinates

Now the volume in phase space is proportional to the Jacobian of the coordinates; therefore, different lattice points in the discretized phase space may represent different volumes. As a consequence, \( P_i^{eq} \) has to be multiplied by this Jacobian and equations like equation (2) have to be modified accordingly. Before we deal with the general case, let us consider the case of polar coordinates.

2.3.1. Polar coordinates. Let the coordinates be \( r, \varphi \), with volume element \( r \, dr \, d\varphi \). For the variable \( \varphi \) the analysis remains unchanged, but for \( r \) we have \( P_i^{eq}/P_{i+1}^{eq} = e^{\epsilon_i/k_B T r}/(r + \ell) \) and equations like equation (2) have to be replaced with equations like

\[
W_{i+1,-} = W_{i,+}e^{\epsilon_i/k_B T r}/(r + \ell).
\]

(13)

Following the steps of section 2.1, instead of equation (11) we now obtain

\[
\Delta r = \Gamma_r \partial[k_B T \log(r \Gamma_r) - E]/\partial r \, \tau + \eta_r,
\]

(14)

where \( \eta_r \) has average 0, variance \( 2k_B T \Gamma_r \tau \) and Gaussian distribution. The replacement of the term \( \log \Gamma_r \) with \( \log r \Gamma_r \) implies a drift towards larger values of \( r \).

It is tempting [19] to attribute the drift towards larger values of \( r \) to the fluctuations of \( \varphi \): if the system moves in phase space by the amount \( r \delta \varphi \) perpendicular to the radial direction, the new value of \( r \) would be \( \sqrt{r^2 + (r \delta \varphi)^2} \approx r [1 + (\delta \varphi)^2/2] \). After a lapse of time \( \tau \) this effect would contribute an increment of \( r \) by the amount \( r (\Delta \varphi)^2/2 = r k_B T \Gamma_r \varphi \). Comparison of this result with equation (14) indicates that this interpretation would be consistent with the principle of detailed balance only if \( \Gamma_r = r^2 \Gamma_r \).

2.3.2. The general case. Let the coordinates be \( v_1, \ldots, v_N \), with volume element \( J(v_1, \ldots, v_N)dv_1, \ldots, dv_N \). Then, when dealing with the transitions of the variable \( v_j \), equation (13) generalizes to

\[
W_{i+1,-} = W_{i,+}e^{\epsilon_i/k_B T J)/(J + \ell \partial J/\partial v_j)}.
\]

(15)

Following the steps of section 2.1, \( \lambda_i \) has an additional term \( [\ell/(2J)]\partial J/\partial v_j \) and equation (14) generalizes to

\[
\Delta v_j = \Gamma_j \partial[k_B T \log(J \Gamma_j) - E]/\partial v_j \, \tau + \eta_j,
\]

(16)

where \( \eta_j \) has average 0, variance \( 2k_B T \Gamma_j \tau \) and Gaussian distribution. An analogous result for macroscopic variables was obtained in [20].

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3. Application—a model for superconductivity

One of the most useful models in the study of dynamic properties of superconductors is the time-dependent Ginzburg–Landau model [21, 22]. In this model the microstate of a superconductor is described by a complex field \( \psi(x, y, z) \), such that \(|\psi(x, y, z)|^2\) is proportional to the density of superconducting electrons at position \((x, y, z)\). Knowledge of the field \( \psi \) enables us to evaluate several measurable quantities, such as the supercurrent density. Since in this model the variable of the problem is itself a field, it may provide an example in which the Langevin approach appears to be more practical than using the Fokker–Planck equation, since the latter is a partial differential equation in a space with infinitely many dimensions.

In most cases, the time-dependent Ginzburg–Landau model is justified only for temperatures very close to the transition temperature. The model was generalized by Kramer and Watts-Tobin [23]; this generalized model is expected to be valid as long as there is local equilibrium. In order to focus on the aspects that we want to illustrate, we deal here with a simplified situation of the Kramer–Watts-Tobin model. We consider a uniform 1D superconductor with periodic boundary conditions and ignore the electromagnetic field. We discretize the system by dividing it into \( N \) segments of equal length and denote by \( \psi_j \) the value of \( \psi \) at segment \( j \). With appropriate normalizations, the energy of the system is given by

\[
E = \sum_{j=1}^{N} \left( -|\psi_j|^2 + \frac{1}{2}|\psi_j|^4 + \xi^2|\psi_j - \psi_{j-1}|^2 \right),
\]

where \( \xi \) is a constant that depends on the material, the temperature, and the length of each segment. If fluctuations are ignored, the evolution of \( \psi_j \) is given by [23]

\[
\frac{u}{\sqrt{1 + \gamma^2|\psi_j|^2}} \left( \frac{d\psi_j}{dt} + \frac{\gamma^2}{2} \frac{d|\psi_j|^2}{dt} \psi_j \right) = (1 - |\psi_j|^2)\psi_j + \xi^2(\psi_{j+1} + \psi_{j-1} - 2\psi_j),
\]

where \( u \) and \( \gamma \) are additional positive constants of the model.

Let us first consider the case \( \gamma^2(\psi_j|^2) \ll 1 \), so that the left-hand side in equation (18) can be approximated by \( u \frac{d\psi_j}{dt} \). In this case it is convenient to express \( \psi_j \) in Cartesian form, \( \psi_j = x_j + iy_j \), and the energy becomes \( \sum_{j=1}^{N} \left[ -(x_j^2 + y_j^2) + (x_j^2 + y_j^2)^2/2 + \xi^2(x_j - x_{j-1})^2 + \xi^2(y_j - y_{j-1})^2 \right] \). Performing the derivatives and separating real and imaginary parts, equation (18) takes the form

\[
\frac{dx_j}{dt} = -\Gamma_x \frac{\partial E}{\partial x_j},
\]

with \( \Gamma_x = 1/(2u) \), and an analogous equation is obtained for \( y_j \). Since \( u \) is constant, we can apply the result (11) with no drift term and conclude that after time \( \tau \) the fluctuating part of the increment of \( x_j \) will have a variance \( k_B T \tau / u \).

Let us now consider the general situation. In this case it is convenient to express \( \psi_j \) in polar form, \( \psi_j = r_j e^{i\varphi_j} \); the energy becomes \( \sum_{j=1}^{N} \left[ -r_j^2 + r_j^2/2 + \xi^2(r_j^2 + r_{j-1}^2 - 2r_jr_{j-1}\cos(\varphi_j - \varphi_{j-1})) \right] \) and the expression in brackets in the left-hand side of equation (18) becomes \([ (dr_j/dt)(1 + \xi^2 r_j^2) + ir_j d\varphi_j/dt )e^{i\varphi_j} \). Multiplying equation (18) by \( e^{-i\varphi_j} \) and taking
the real part we obtain the evolution of $r_j$,
\[ \frac{dr_j}{dt} = -\frac{1}{2u\sqrt{1 + \gamma^2 r_j^2}} \frac{\partial E}{\partial r_j}; \]  
(20)

taking the imaginary part gives the evolution of $\varphi_j$,
\[ \frac{d\varphi_j}{dt} = -\frac{\sqrt{1 + \gamma^2 r_j^2}}{2ur_j^2} \frac{\partial E}{\partial \varphi_j}. \]  
(21)

These equations are in the form of equation (1), with $\Gamma_r = \frac{1}{2u\sqrt{1 + \gamma^2 r_j^2}}$ and $\Gamma_\varphi = \sqrt{1 + \gamma^2 r_j^2}/(2ur_j^2)$. In the extreme case $\gamma r_j \gg 1$, $\Gamma_r \approx \frac{1}{2u\gamma r_j}$ and $\Gamma_\varphi \approx \gamma/(2ur_j)$.

Since in this limiting situation $\gamma r_j \gg 1$, the correction terms $\log(r)$ are not required and the formalism developed in section 2.3.1 can be applied without drift terms. For general $\gamma$, thermal fluctuations add a drift to equation (20) and lead to

\[ \Delta r_j = \Gamma_r \left[ k_B T \left( \frac{1}{r_j} - \frac{\gamma^2 r_j}{1 + \gamma^2 r_j^2} \right) \frac{\partial E}{\partial r_j} \right] \tau + \eta_r = \Gamma_r \left[ k_B T \frac{r_j}{1 + \gamma^2 r_j^2} \frac{\partial E}{\partial r_j} \right] \tau + \eta_r, \]  
(22)

where $\eta_r$ is the usual Langevin term with variance $2k_B T \Gamma_r \tau$.

It should be emphasized that equation (22) (including the drift) is an extension of equation (20) and not a modification of it. As an illustration of this statement, let us focus on the case $\gamma = 0$ already considered in equation (19). In this case the drift term becomes $k_B T/r_j \neq 0$ and $\Gamma_r$ becomes $1/(2u \gamma)$, i.e. $\Gamma_r = \Gamma_x$. Moreover, let us for a moment leave the KWT model aside and consider the toy model $E = \sum_{j=1}^N r_j^2 = \sum_{j=1}^N (x_j^2 + y_j^2)$, i.e., we just have $u d\psi_j/dt = -\psi_j$ instead of equation (18) and $u dr_j/dt = -r_j$ instead of equation (20).

It follows that if the drift term $k_B T/r_j$ were not present, the evolution equations for $x_j$, $y_j$ and $r_j$ (including fluctuations) would all become identical and we would therefore have $\langle r_j^2 \rangle = \langle x_j^2 \rangle = \langle y_j^2 \rangle$, whereas the true relationship is $\langle r_j^2 \rangle = \langle x_j^2 + y_j^2 \rangle = 2\langle x_j^2 \rangle$.

4. Conclusion

We have developed a simple method that enables us to derive the Langevin and drift terms for systems with the random-walk type of evolution. The concepts of probability theory that we have invoked are intuitive and elementary (in the ‘language’ used by undergraduate physics textbooks). This method is particularly useful when the dynamics leads to an anisotropic phase space or when the evolution is naturally expressed in curvilinear coordinates.

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Appendix A. Itô or Stratonovich?

We first note that the two terms in equation (11) are not of comparable sizes. The first is \( O(\tau) \), whereas \( \eta \) is \( O(\tau^{1/2}) \). This does not mean that \( \eta \) is more important, since it tends to cancel in the long run, whereas the first term persists.

The next question concerns the precise value of \( x \) at which equation (11) should be evaluated. Should it be the initial value, \( x = x_{\text{in}} \), the final value \( x = x_{\text{in}} + \Delta x \), or some intermediate value? For the first term this question is irrelevant, since the change in the value of this term is \( O(\tau \Delta x) \) and its contribution vanishes in the limit \( \tau \to 0 \) (even after noting that decreasing the time interval by some factor increases the number of intervals by the same factor). This is not the case for the choice of the \( x \)-dependent variance of \( \eta \).

The Itô procedure evaluates the variance at \( x = x_{\text{in}} \). \( \eta \) has a symmetric distribution and \( \langle \eta \rangle = 0 \). The Stratonovich procedure evaluates the variance at the middle of the interval, \( x = x_{\text{in}} + \Delta x / 2 \). In order to distinguish between the two procedures, we denote the respective random terms by \( \eta_i \) and \( \eta_S \). In order to fix ideas, let us explore the case where \( \Gamma(x) \) is an increasing function of \( x \). Since the variance is evaluated at \( x \approx x_{\text{in}} + \eta_S / 2 \), it means that if \( \eta_S > 0 \) (respectively \( \eta_S < 0 \)), then \( \eta_S / \eta_i > 1 \) (respectively \( \eta_S / \eta_i < 1 \)). Qualitatively, this means that the distribution of \( \eta_S \) will have a longer tail than that of \( \eta_i \) in the positive direction and a shorter tail in the negative direction.

In more quantitative terms, we can establish a one to one correspondence between the values of \( \eta_S \) and those of \( \eta_i \), such that

\[
\eta_S \approx \left[ \frac{\Gamma(x_{\text{in}} + \eta_S / 2)}{\Gamma(x_{\text{in}})} \right]^{1/2} \eta_i \approx \left( 1 + \Gamma' \eta_S / 2 \Gamma \right)^{1/2} \eta_i \approx \left( 1 + \Gamma' \eta_i / 4 \Gamma \right) \eta_i = \eta_i + \Gamma' \eta_i^2 / 4 \Gamma, \tag{A.1}
\]

where we have written \( \Gamma \) as shorthand for \( \Gamma(x_{\text{in}}) \) and \( \Gamma' \) for \( d\Gamma/dx \) at \( x = x_{\text{in}} \). The approximations in (A.1) are \( \Delta x \approx \eta_S \), expansions to first order in \( \Delta x \), and \( \eta_S \eta_i \approx \eta_i^2 \). The important consequence is that for sufficiently small \( \tau \) we have

\[
\langle \eta_S \rangle = \langle \eta_i \rangle + (\Gamma' / 4 \Gamma) \langle \eta_i^2 \rangle = k_B T \Gamma' \tau / 2. \tag{A.2}
\]

This term is not negligible and does not cancel in the long run.

In a didactic article, van Kampen [24] explains how to translate between the Itô and the Stratonovich procedures. He advocates the use of a master equation rather than a Langevin approach, so that the Itô–Stratonovich dilemma never arises. Lançon et al performed an experiment in which colloidal particles diffuse in a medium with position-dependent diffusion coefficient, so that \( \langle \eta_S \rangle \neq \langle \eta_i \rangle \). In their case they found that \( \Gamma(x) \) has to be evaluated at \( x = x_{\text{in}} \) [25].

In order to judge what is the appropriate procedure for equation (11) in our case, we will evaluate \( \langle \eta \rangle \). Since the difference between the two procedures depends on \( w(x) \) and not on \( \lambda \), we are free to take \( \lambda \equiv 1 \) (we may imagine that \( E - k_B T \log \Gamma \) is constant) and are left with a random-walk problem in which each step is equally probable for both directions. Let the system be initially at \( x = x_{\text{in}} \); by definition, the probability distribution for \( \eta \) is the probability distribution for \( x = x_{\text{in}} \) after time \( \tau \).

Let \( P_i \) be the probability for finding the system at \( x = i \ell \) at some moment. The change of probability after time \( \delta t \) will be \( \delta P_i = (w_{i-1} P_{i-1} - 2 w_i P_i + w_{i+1} P_{i+1}) \delta t \). Or, defining \( \rho_i = w_i P_i \),

\[
\delta \rho_i = w_i (\rho_{i-1} - 2 \rho_i + \rho_{i+1}) \delta t. \tag{A.3}
\]

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Figure A.1. Deviation of the probability density from the Itô distribution. The unit of length can be chosen arbitrarily. The unit of time equals the square of the length unit divided by \( k_B T \Gamma(x_{\text{in}}) \). The probability density is in units of \( d \log \Gamma/dx \).

In order to use the central limit theorem, we require \( \delta t/\tau \to 0 \) and we pass to a continuous model. Equation (A.3) becomes the diffusion equation

\[
\frac{\partial \rho}{\partial t} = k_B T \Gamma(x) \frac{\partial^2 \rho}{\partial x^2}.
\]  

(A.4)

In order to pass from equations (A.3) to (A.4) we have expanded \( \rho(x) \) to \( O(\ell^2) \) and used the definition of \( \Gamma \). Equation (A.4) may be regarded as our master equation.

Let us take the initial value \( \rho(x, 0) = w(x_{\text{in}}) \delta(x-x_{\text{in}}) \). If in equation (A.4) \( \Gamma(x) \) were substituted by the constant \( \Gamma(x_{\text{in}}) \), the solution of the diffusion equation would be

\[
\rho^{(0)}(x, t) = \frac{w(x_{\text{in}})}{2 \sqrt{\pi k_B T \Gamma(x_{\text{in}}) t}} \exp\left[ -\frac{(x-x_{\text{in}})^2}{4 k_B T \Gamma(x_{\text{in}}) t} \right],
\]  

(A.5)

which is just the Itô distribution multiplied by \( w(x_{\text{in}}) \). We now deal with equation (A.4) by means of the approximation

\[
\frac{\partial \rho}{\partial t} = k_B T \left[ \Gamma(x_{\text{in}}) + \Gamma(x) - \Gamma(x_{\text{in}}) \right] \frac{\partial^2 \rho}{\partial x^2} \approx k_B T \Gamma(x_{\text{in}}) \frac{\partial^2 \rho}{\partial x^2} + k_B T \Gamma'(x-x_{\text{in}}) \frac{\partial^2 \rho^{(0)}}{\partial x^2}.
\]  

(A.6)

This nonhomogeneous equation is solved using the Green function of the diffusion equation [26]. We obtain that the deviation of the probability distribution from the Itô distribution is \( \Delta P(x, \tau) = (d \log \Gamma/dx)(-6\phi + \phi^3) \exp(-\phi^2/4)/(16\sqrt{\tau}) \), where \( \phi = (x-x_{\text{in}})/\sqrt{k_B T \Gamma(x_{\text{in}}) \tau} \) and the derivative is evaluated at \( x = x_{\text{in}} \). A plot of this deviation is shown in figure A.1 (for any value of \( \tau \) for which the approximations in equation (A.6) are justified).

The deviation \( \Delta P \) enhances the positive tail of the distribution of \( \eta_I \) and hinders the negative tail, as in the case of \( \eta_S \). However, the key feature is that \( \langle \eta \rangle \) is not affected by
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\[ \Delta \mathcal{P}; \text{ therefore, } \eta \text{ has the appropriate distribution for our problem and the Itô procedure should be used. Also } \langle \eta^2 \rangle \text{ is not affected by } \Delta \mathcal{P}. \text{ It is interesting to note that, no matter how small } \tau \text{ is, there are always values of } x \text{ where } \Delta \mathcal{P} \text{ remains finite; however, the statistical weight of } \Delta \mathcal{P} \text{ does become negligible in the limit of small } \tau. \]

Appendix B. Linear transformation of variables

Let \( x_1, \ldots x_N \) be the original set of variables for which the evolution of the system is known. Let us restrict ourselves to cases in which the coefficients \( \Gamma_j \) are independent of the coordinates, so that \( G_j = E \). Let \( u_1, \ldots u_N \) be a new set of variables, defined by means of a linear transformation

\[
\begin{align*}
  u_i &= \sum_{j=1}^{N} C_{ij} x_j / \sqrt{\Gamma_j}, \\
  \end{align*}
\]

where \( C_{ij} \) are the elements of a constant orthogonal matrix \( C \); the purpose of the factor \( \sqrt{\Gamma_j} \) is to compensate for the anisotropy of phase space.

Substituting equation (12) into (B.1) we obtain

\[
\Delta u_i = -\sum_{j=1}^{N} C_{ij} \sqrt{\Gamma_j} \frac{\partial E}{\partial x_j} \tau + \xi_i,
\]

where \( \xi_i = \sum_{j=1}^{N} C_{ij} \eta_j / \sqrt{\Gamma_j} \) is a fluctuating term with zero average and Gaussian distribution. Its variance is

\[
\sum_{j=1}^{N} C_{ij}^2 \langle \eta_j^2 \rangle / \Gamma_j = 2k_B \tau \sum_{j=1}^{N} C_{ij}^2 = 2k_B \tau,
\]

where we have used the property that \( \eta_j \) and \( \eta_{j'} \) are not correlated for \( j \neq j' \) and the orthogonality of \( C \). For \( i \neq i' \) we have

\[
\langle \xi_i \xi_{i'} \rangle = \sum_{j,j'=1}^{N} C_{ij} C_{i'j'} \langle \eta_j \eta_{j'} \rangle / \sqrt{\Gamma_j \Gamma_{j'}} = 2k_B \tau \sum_{j=1}^{N} C_{ij} C_{i'j} = 0,
\]

where we have used again \( \langle \eta_j \eta_{j'} \rangle = 2k_B \tau \Gamma_j \delta_{jj'} \) and orthogonality of \( C \).

Since \( x_j = \sqrt{\Gamma_j} \sum_{i=1}^{N} C_{ji}^{-1} u_i = \sqrt{\Gamma_j} \sum_{i=1}^{N} C_{ij} u_i \), \( \partial x_j / \partial u_i = \sqrt{\Gamma_j} C_{ij} \). Therefore,

\[
\frac{\partial E}{\partial u_i} = \sum_{j=1}^{N} \frac{\partial x_j}{\partial u_i} \frac{\partial E}{\partial x_j} = \sum_{j=1}^{N} \sqrt{\Gamma_j} C_{ij} \frac{\partial E}{\partial x_j}.
\]

Comparing equations (B.5) and (B.2) we finally obtain

\[
\Delta u_i = -\frac{\partial E}{\partial u_i} \tau + \xi_i.
\]

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