FUNCTIONAL INTEGRAL AND OPERATOR FORMALISMS FOR A MODIFIED LANGEVIN EQUATION

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We construct functional integral and operator formalisms for the stochastic process generated by a modified Langevin equation which contains a white noise and an independent markovian process taking discrete values.

Functional integral [1–4] and operator formalisms [5–7] have been developed for the markovian processes described by Langevin equations. We study here the stochastic process generated by a modified Langevin equation and we treat the case of one slow variable to simplify the discussion (the generalization to several slow variables is straightforward). We consider the stochastic process $q(t)$ defined by the Langevin equation $\dot{q}(t) + A(q(t), m(t)) = f(t)$, where $f(t)$ is a gaussian white noise with $\{f(t)\} = 0$ and correlation $\{f(t)f(t')\} = c\,\delta(t - t')$ and $m(t)$ is an independently defined markovian process taking values $\nu = 1, 2, ..., N$ and characterized by the $N \times N$ matrix $M_{\mu\nu}$ in the sense that if $m(t) = \mu$ the probability that $m(t + s) = \nu$ is $[\exp(-sM)]_{\mu\nu}$. The process $(q(t), m(t))$ is markovian and the conditional probability $P(q, \nu, t; q_0, \nu_0, t_0) = W^\nu(q, t)$ satisfies (we keep the initial conditions at t_0 fixed) a Fokker–Planck equation that we can determine discretizing the original Langevin equation putting $t_n = t_0 + n\epsilon$, $n \in \bar{N} = (0, 1, 2, ...)$ and taking at the end $\epsilon \to 0$. We divide the real axis in cells $[j\eta, (j + 1)\eta)$ and we say $q(t) = j\eta$ if $j\eta \leqslant q(t) < (j + 1)\eta$. Putting $q^{(n)} = q(t_n)$, $f^{(n)} = f(t_n)$, $m^{(n)} = m(t_n)$, the Langevin equation is

$$q^{(n)} = q^{(n-1)} + \epsilon(f^{(n-1)} - A(q^{(n-1)}, m^{(n-1)}))\,, \tag{1}$$

and $\{f(t)f(t')\}$ becomes $\{f^{(n)}f^{(n')}\} = (c/\epsilon)\delta_{nn'}$ and we can then replace $f^{(n)}$ by a random variable taking values $\pm(c/\epsilon)^{1/2}$ with probability 1/2. In the discretization we note $(k, \nu, n|0) = W^\nu(q, t)$ which means that at $t = t_0 + n\epsilon$ one has $q(t) = k\eta$, $m(t) = \nu$. Then

$$(k, \nu', n + 1|0) = \sum_{j,\nu} p_{j\nu,k\nu'}(j, \nu, n|0)\,, \tag{2}$$

where $p_{j\nu,k\nu'}$ is the probability of going in the interval of time ϵ from (j, ν) to (k, ν'). One has $p_{j\nu,k\nu'} = p_{jk}^{(\nu)}(\delta_{\nu\nu'} - \epsilon M_{\nu\nu'})$, where $p_{jk}^{(\nu)}$ is the probability that $q(t + \epsilon) = k\eta$ if $q(t) = j\eta$, $m(t) = \nu$. Observing that the term $\epsilon f^{(n-1)}$ in eq. (1) just causes a jump from cell j to $j - 1$ or $j + 1$, in both cases with probability 1/2 (this is the motivation to choose cells of length η) one can write $p_{jk}^{(\nu)} = \frac{1}{2}(\bar{p}_{j,k-1}^{(\nu)} + \bar{p}_{j,k+1}^{(\nu)})$, where $\bar{p}_{jk}^{(\nu)}$ is defined as $p_{jk}^{(\nu)}$ but when $f(t)$ does not act. We note now that

$$|\epsilon A(j\eta, \nu)/\eta| = |A(j\eta, \nu)/c^{1/2}|\epsilon^{1/2} \ll 1\,, \qquad \epsilon \to 0\,,$$

and then if $A(j\eta, \nu) > 0$ (if $A(j\eta, \nu) < 0$ the argument is similar) the term $-\epsilon A(j\eta, \nu)$ in eq. (1) causes a change to cell $j-1$ if $q(t)$ is in the subinterval of length $\epsilon A(j\eta,\nu)$ at the left of $[j\eta,(j+1)\eta)$ and no change of cell if $q(t)$ is in the complement, consequently

$$\bar{p}^{(\nu)}_{jk} = (1-\epsilon A(j\eta,\nu)/\eta)\,\delta_{jk} + (\epsilon A(j\eta,\nu)/\eta)\,\delta_{j,k+1}\,.$$

We can now compute $p_{j\nu,k\nu'}$ and replace it in eq. (2). In the limit $\epsilon\to 0$ one has

$$\eta^{-2}\,[(k+1,\nu',n|0) - 2(k,\nu',n|0) + (k-1,\nu',n|0)] \to (\partial^2/\partial q^2)W^{\nu'}(q,t)\,,$$

$$\epsilon^{-1}\,[(k,\nu',n+1|0) - (k,\nu',n|0)] \to \dot{W}^{\nu'}(q,t)\,,$$

etc., and one obtains

$$\dot{W}^{\nu}(q,t) = (\partial/\partial q)(A(q,\nu) + \tfrac{1}{2}c(\partial/\partial q))W^{\nu}(q,t) - \sum_{\nu'} M_{\nu'\nu}W^{\nu'}(q,t)\,. \tag{3}$$

An operator formalism can now be introduced which is the analogue of quantum mechanics with spin and for which we use the usual notation. Let $\mathcal{H}_1$ be a Hilbert space in which the operators $\hat{q}_1$, $\hat{p}_1$ act with commutation relations $[\hat{q}_1,\hat{p}_1] = \mathrm{i}$, and E a vector space of dimension N with the orthonormal basis $|\nu\rangle$, $1\leqslant\nu\leqslant N$. In $\mathcal{H}_1$ we have the basis $|q\rangle$, $\hat{q}_1|q\rangle = q|q\rangle$ and the basis $|p\rangle$, $\hat{p}_1|p\rangle = p|p\rangle$, both normalized to a δ-function. Consider the tensor product $\mathcal{H} = \mathcal{H}_1\otimes E$ and define in $\mathcal{H}$ the operators $\hat{q}\equiv\hat{q}_1\otimes I_E$, $\hat{p}\equiv\hat{p}_1\otimes I_E$ (I_E = identity in E). The vectors

$$|q,\nu\rangle \equiv |q\rangle\otimes|\nu\rangle\,,\quad \hat{q}|q,\nu\rangle = q|q,\nu\rangle\,,\quad \langle q',\nu'|q,\nu\rangle = \delta_{\nu\nu'}\delta(q-q')\,,$$

form a basis in $\mathcal{H}$, as well as $|p,\nu\rangle\equiv|p\rangle\otimes|\nu\rangle$, and $\langle q,\nu|p,\nu'\rangle = \delta_{\nu\nu'}(2\pi)^{-1/2}\exp(\mathrm{i}pq)$. We define in $\mathcal{H}$ the "hamiltonian" operator $\hat{H}$ with matrix elements

$$\langle q',\nu'|\hat{H}|q,\nu\rangle = \delta_{\nu\nu'}(-\tfrac{1}{2}\mathrm{i}c\langle q'|\hat{p}_1^2|q\rangle - A(q,\nu)\langle q'|\hat{p}_1|q\rangle) - \mathrm{i}M_{\nu\nu'}\,,$$

and the evolution operator $U(t',t)$ by

$$\mathrm{i}\partial U(t',t)/\partial t' = \hat{H}U(t',t)\,,\quad U(t,t) = 1\,.$$

Then one easily checks that

$$P(Q,\nu,t;Q_0,\nu_0,t_0) = \langle Q,\nu|U(t,t_0)|Q_0,\nu_0\rangle\,.$$

We can write a functional integral representation for P. Using $\Sigma_\mu\int \mathrm{d}q\,|q,\mu\rangle\langle q,\mu| = 1$ one has ($t_j = t_0 + j\epsilon$, $t_{n+1} = t$)

$$\langle Q,\nu|U(t,t_0)|Q_0,\nu_0\rangle = \sum_{\mu_1\ldots\mu_n}\int_{\substack{q_0=Q_0\\ \mu_0=\nu_0}}^{\substack{q_{n+1}=Q\\ \mu_{n+1}=\nu}} \prod_{i=1}^{n}\mathrm{d}q_i \prod_{j=1}^{n+1}\langle q_j,\mu_j|U(t_j,t_{j-1})|q_{j-1},\mu_{j-1}\rangle\,. \tag{4}$$

But from $U(t_j,t_j-1) = 1-\mathrm{i}\epsilon\hat{H}$ (only terms up $\mathrm{O}(\epsilon)$ are needed in the limit $n\to\infty$, $\epsilon\to 0$) and using the known matrix elements of $\hat{H}$ we obtain for eq. (4)

$$\sum_{\mu_1\ldots\mu_n}\int\prod_{i=1}^{n}\mathrm{d}q_i\prod_{j=1}^{n+1}\frac{\mathrm{d}p_j}{2\pi}\prod_{j=1}^{n+1}\exp\mathrm{i}\epsilon[p_j(q_j-q_{j-1})/\epsilon - h_{\mu_j\mu_{j-1}}(p_j,q_{j-1})]\,, \tag{5}$$

where $h_{\mu\nu}(p,q)\equiv\delta_{\mu\nu}(-\tfrac{1}{2}\mathrm{i}cp^2 - pA(q,\nu)) - \mathrm{i}M_{\nu\mu}$. If we define the $N\times N$ matrix $\tilde{h}(p,q)$ of elements $h_{\mu\nu}(p,q)$ then the product of exponentials in (5) (each term is needed only up to $\mathrm{O}(\epsilon)$) is the element $(\mu_{n+1}\mu_0)$ of a product of matrices and in the limit $n\to\infty$ one can formally write the functional integral

$$P(Q,\nu,t;Q_0,\nu_0,t_0) = \int_{\mu_0=\nu_0}^{\mu_{n+1}=\nu}\mathcal{D}q\mathcal{D}p\;T\exp\mathrm{i}\int_{t_0}^{t}\mathrm{d}\tau\,[p\dot{q} - \tilde{h}(p(\tau),q(\tau))]\cdot\delta(q(t)-Q)\,\delta(q(t_0)-Q_0)\Big|_{\mu_{n+1}\mu_0}\,, \tag{6}$$

where T means that when discretizing eq. (6) the product of matrices is to be done chronologically, i.e. as in (5) which is the definition of eq. (6). We note that in eq. (6) the discretization of functions of q is in the prepoint as indicated in (5), this means that we are using the $\gamma(0)$ discretization [3,8] and we should write $\gamma(0)$ as a subscript in eq. (6), but as we shall only use this discretization here we omit the $\gamma(0)$. We define now the operators $\hat{q}(t) = U^{-1}(t)\hat{q}U(t)$, $\hat{p}(t) = U^{-1}(t)\hat{p}U(t)$, where $U(t) \equiv U(t,0)$ and the vectors

$$|Q_0, \nu_0, t_0\rangle^{\mathrm{R}} \equiv U^{-1}(t_0)|Q_0, \nu_0\rangle\,, \qquad \langle \mathrm{L}| \equiv \sum_\nu \int \mathrm{d}q\, \langle q, \nu|\,.$$

The conservation of probability implies $\langle \mathrm{L}|U(t) = \langle \mathrm{L}|$ for all t, where one has used $\Sigma_\mu M_{\nu\mu} = 0$. One shows in the same way as we did for eq. (6) that ($t > t_i'$, $t_j > t_0$, $t_i' \neq t_j$)

$$\langle \mathrm{L}|T\hat{p}(t_1') \ldots \hat{p}(t_m')\hat{q}(t_1) \ldots \hat{q}(t_n)|Q_0, \nu_0, t_0\rangle^{\mathrm{R}} = \int_{\mu_0=\nu_0} \mathcal{D}q\mathcal{D}p\; Tp(t_1') \ldots q(t_n) \exp \mathrm{i} \int \mathrm{d}\tau\, (p\dot{q} - \tilde{h}) \cdot \delta(q(t_0) - Q_0), \tag{7}$$

where T in the left-hand side is the usual chronological product. Note that the right-hand side of eq. (7) (which we denote by $\langle p(t_1') \ldots q(t_n)\rangle$) is, before the limit $n \to \infty$, a matrix element $(\mu_{n+1}\mu_0)$ where $\mu_0 = \nu_0$ is fixed, and we must sum over μ_{n+1} due to the definition of $\langle \mathrm{L}|$. The functional integrals in eqs. (6) and (7) are found in quantum mechanics in the treatment of problems with spin [9] and have been studied in that context in ref. [10]; they are known in mathematics as product integrals. When only $q(t_i)$ is present the left-hand side of eq. (7) is (putting $t_{n+1} = t_0$, $q_{n+1} = Q_0$, $\nu_{n+1} = \nu_0$ and supposing $t_1 \geqslant t_2 \ldots \geqslant t_n \geqslant t_0$)

$$\sum_\nu \int \mathrm{d}q\, \langle q, \nu|U(t_1)U^{-1}(t_1)\hat{q}U(t_1) \ldots U^{-1}(t_n)\hat{q}U(t_n)U^{-1}(t_0)|Q_0, \nu_0\rangle$$

$$= \sum_{\nu_1 \ldots \nu_n} \int \prod_{i=1}^{n} \mathrm{d}q_i \prod_{j=1}^{n} \langle q_j, \nu_j|\hat{q}U(t_j, t_{j+1})|q_{j+1}, \nu_{j+1}\rangle\,. \tag{8}$$

Using $\langle q_j, \nu_j|\hat{q} = q_j\langle q_j, \nu_j|$ one obtains from eq. (8) that

$$\langle q(t_1) \ldots q(t_n)\rangle = \int \prod_{i=1}^{n} \mathrm{d}q_i\, q_1 \ldots q_n \sum_{\nu_1 \ldots \nu_n} \prod_{j=1}^{n} P(q_j, \nu_j, t_j; q_{j+1}, \nu_{j+1}, t_{j+1})\,. \tag{9}$$

But $\Sigma\, \Pi\, P(q_j, \nu_j, t_j; q_{j+1}, \nu_{j+1}, t_{j+1})$ is just the joint probability $W_n(q_1, t_1; \ldots; q_n, t_n)$ (for fixed initial conditions Q_0, ν_0 at time t_0) of the non-markovian process $q(t)$ and then $\langle q(t_1) \ldots q(t_n)\rangle$ are correlation functions. In order to interpret eq. (7) when $p(t)$ is also present we modify in our original Langevin equation the drift $A(q(t), m(t))$ to $A(q(t), m(t)) + K(t)$, this modifies $\hat{H}$ to $\hat{H}' = \hat{H} - K(t)\hat{p}$ and then $h_{\mu_j\mu_{j-1}}(p_j, q_{j-1})$ in (5) is replaced by $h'_{\mu_j\mu_{j-1}} = h_{\mu_j\mu_{j-1}} - \delta_{\mu_j\mu_{j-1}}K(t_{j-1})$.

Let $\langle q(t_1) \ldots q(t_n)\rangle_K$ be the new correlation functions, then from eq. (7) with $\tilde{h}$ replaced by $\tilde{h}'$ we obtain

$$(1/\mathrm{i})(\delta/\delta K(t''))\langle q(t')\rangle_K = \langle \mathrm{L}|T\hat{p}(t'')\hat{q}(t')|Q_0, \nu_0, t_0\rangle^{\mathrm{R}} = \langle p(t'')q(t')\rangle\,, \tag{10}$$

which shows that $\langle p(t'')q(t')\rangle$ is the linear response function corresponding to a modification of the drift (the same applies for several $p(t)$). Obviously eq. (7) vanishes when one has only $p(t_i')$ or when a time t_i' is greater than all t_j (causality). We remark that in eq. (10) the T-product is not defined at $t'' = t'$ while $\langle p(t'')q(t')\rangle$, being defined by the functional integral in eq. (7), is defined and due to the $\gamma(0)$ discretization [3] we are using has the value $\langle p(t'')q(t')\rangle$, $t'' \to t' + 0$, that is, it vanishes. In general, when in $\langle p(t_1') \ldots q(t_n)\rangle$ a time $t_i' = t_j$, the value is the limit $t_i' \to t_j + 0$. One can now use operator or functional integral techniques to study the process $q(t)$. In particular, a systematic perturbation expansion can be obtained in the operator formalism using the Wick theorem [7,11], or more easily with functional integral techniques [4] starting from the generating functional $Z[j, j^*]$ for correlation and response functions which is

$$Z[j,j^*] = \int_{\mu_0=\nu_0} \mathcal{D}q\mathcal{D}p \, T\exp \mathrm{i} \int_{t_0}^{\infty} \mathrm{d}\tau \, [p\dot{q} - \tilde{h} + j(\tau)q(\tau) + j^*(\tau)p(\tau)] \cdot \delta(q(t_0) - Q_0) \,, \tag{11}$$

where the source terms correspond to changing $\hat{H}$ to $\hat{H} - j(t)\hat{q} - j^*(t)\hat{p}$. The averaging over the initial conditions at t_0 is easily done: if one is given the probability $b(\nu, q)$, $\Sigma_\nu \int \mathrm{d}q \, b(\nu, q) = 1$, at time t_0, this just changes the vector $|Q_0, \nu_0, t_0\rangle^{\mathrm{R}}$ to $\Sigma_\nu \int \mathrm{d}q \, b(\nu, q)|q, \nu, t_0\rangle^{\mathrm{R}}$. Applications of the present formalism will be presented elsewhere.

Previous works on particular processes of the type we consider here can be found in refs. [12,13]. The process generated by the Langevin equation without white noise ($f(t) = 0$) is treated in detail in ref. [14].

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