To be submitted to
Physics Letters A

ISTITUTO NAZIONALE DI FISICA NUCLEARE
Laboratori Nazionali di Frascati

LNF-78/19(P)
2 Maggio 1978

E. Etim and C. Basili: ON THE PATH INTEGRAL SOLUTIONS OF THE MASTER EQUATION.

Servizio Documentazione
dei Laboratori Nazionali di Frascati
Cas. Postale 13 Frascati (Roma)

Laboratori Nazionali di Frascati
Servizio Documentazione

LNF-78/19(P)
2 Maggio 1978

E. Etim and C. Basili[(*)]: ON THE PATH INTEGRAL SOLUTIONS OF THE MASTER EQUATION.

ABSTRACT. -

The Lagrangian in the path integral solution of the master equation of a stationary Markof process is derived by application of the Ehrenfest-type theorem of quantum mechanics and the Cauchy method of finding inverse functions. Applied to the non-linear Fokker-Planck equation we reproduce the result obtained by integrating over Fourier series coefficients and by other methods.

(*) Postal Address: Istituto di Matematica, Università di Roma

The Fokker-Planck equation

$$\frac{\partial w(q,t)}{\partial t} = \sum_{n=1}^{2} \left(\frac{\partial}{\partial q}\right)^n \left[T_n(q) W(q,t) \right] \qquad (1)$$

has the same mathematical structure as the Schrödinger equation. Attempts to formulate and solve it with methods that have proven successful for the Schrödinger equation, not last that of path integrals, start from this observation[1-3]. The use of path integrals in non-equilibrium thermodynamics is not just an elegant mathematical machinery. The Onsager-Machlup principle[4] extended also to non-linear processes leads naturally to it, allowing one to seek solutions of the master equation, as well as of eq. (1), in the form

$$W(q(t)) = \int \mathscr{D}(q(t)) \exp\left(\int_0^t d\tau \; L(q, \dot{q})\right) \qquad (2)$$

where $L(q, \dot{q})$ is the thermodynamic Lagrangian and the integration in eq. (2) is over all paths from $q=0$ at time $t=0$ to $q(t)$ at time t. The problem of determining the Lagrangian is essentially that of finding the evolution equation for the macrovariable $q=q(t)$ whose probability distribution satisfies eq. (1) or the master equation[5]. The way from eq. (1) to the deterministic equation usually involves approximations on account of which there is a general lack of agreement on the exact structure of the Lagrangian[6]. Recently Dekker[6] has applied the interesting method of integrating over the Fourier expansion coefficients of $q(t)$ to determine the solution of eq.(1) starting from an action of the general form

$$A(t) = \int_0^t d\tau \left(\frac{1}{2} (\dot{q}(\tau) - \alpha(q))^2 + \gamma(q)\right) \qquad (3)$$

The Fourier series method has the advantage of being applicable to both differentiable and non-differentiable paths but it is a little too technical for the problem at hand. The purpose of this note is to show that the Ehrenfest-type theorem of quantum mechanics and the Cauchy integral method of finding inverse functions can be used to standardize the construction of the thermodynamic Lagrangian directly from the differential operator in the Kramers-Moyal expansion[7]. For the technicalities of regulating the action integral one can with a known Lagrangian use the Fourier series expansion.

Consider the master equation

$$\frac{\partial W(q,t)}{\partial t} = -\frac{1}{\alpha}\int du\,(1-e^{-iup})\;T(u,q)W(q,t) \equiv \mathcal{M}(q,\frac{\partial}{\partial q})W(q,t)$$
$$p = -i\alpha\frac{\partial}{\partial q} \qquad (4)$$

for a stationary non-equilibrium Markof process. $T(u,q)$ is the transition probability per unit time and α is an expansion parameter which fixes the extension of the physical system; $\alpha \longrightarrow 0$ in the thermodynamic limit. Let $W_0(q) = V_0^2(q)$ be the (in general degenerate) vacuum ($\equiv$ equilibrium) solution of the eigenvalue equation

$$\mathcal{M}(q, \frac{\partial}{\partial q})W_n(q,t) = -\lambda_n W_n(q,t); \quad n = 0, 1, 2.... \qquad (5)$$

We define the Hamiltonian $H(p,q)$ for the time evolution of the states

$$\varphi_n(q,t) = V_0^{-1}(q)\,W_n(q,t) \qquad (6)$$

by

$$H(p,q) = i\,V_0^{-1}(q)\,\mathcal{M}(q,\frac{\partial}{\partial q})\,V_0(q) \qquad (7)$$

Making use of the Kramers-Moyal expansion one obtains from eq. (7) the equation of motion for $q(t)$ by eliminating p from Hamilton's equations

$$\frac{\partial H(p,q)}{\partial p} = \dot{q} = \sum_{n=1}^{\infty} n\,a_n\,(q)(ip)^{n-1} \qquad (8a)$$

$$\frac{\partial H(p,q)}{\partial q} = -\dot{p} = -i\sum_{n=0}^{\infty} a_n'(q)(ip)^n \qquad (8b)$$

where

$$a_n(q) = \frac{1}{\alpha} V_o^{-1}(q) \sum_{\ell=n}^{\infty} \binom{\ell}{n} \left(\frac{d}{dq}\right)^{\ell-n} (T_\ell(q) V_o(q)) \alpha^{\ell-n} \tag{9a}$$

$$T_n(q) = \frac{(-)^n}{n!} \int du\, u^n\, T(u,q) \tag{9b}$$

We use prime to denote differentiation with respect to q and dot for differentiation with respect to t. We assume that the series in eqs. (8) converge uniformly in $q \neq 0$ and that for all q, $a_2(q) \neq 0$.

Under these assumptions eq. (8a) can be inverted to solve for p as a function of $\dot{q}$ and q by means of the Cauchy integral[8]

$$p = \frac{1}{2\pi i} \oint \frac{z\, dz}{\dot{q}(z) - \dot{q}(p)} \left(\frac{d\dot{q}(z)}{dz}\right) \tag{10}$$

where the contour is in the p-plane and encircles the point $p(\dot{q})$ counterclock wise.

The coefficients of the series expansion of p(q) about $\dot{q} = \dot{q}_o = a_1(q)$ i. e.

$$p(\dot{q}) = \sum_{m=1}^{\infty} b_m(q)(\dot{q} - a_1(q))^m \tag{11}$$

are from eq. (10)

$$b_m(q) = \frac{1}{m!} \left[\frac{d^{m-1}}{dp^{m-1}} \left(\frac{p}{\dot{q}(p) - a_1(q)} \right)^m \right]_{p=0} \tag{12}$$

and can be explicitly computed by substituting for $\dot{q}(p)$ from eq. (8a). A few of them are given below

$$b_1(q) = -i/2\, a_2(q) \tag{13a}$$

$$b_2(q) = 3\, i\, a_3/8\, a_2^3 \tag{13b}$$

$$b_3(q) = -i\,(9\, a_3^2 - 4 a_2\, a_4/16\, a_2^5 \tag{13c}$$

$$b_4(q) = -5i(-27\, a_3^3 + 24\, a_2 a_3 a_4 - 4 a_2^2 a_5)/(2a_2)^7 \tag{13d}$$

$$b_5(q) = i(-1134\, a_3^4 + 304\, a_2 a_3 a_4 - 192\, a_2^2 a_4^2 - 360\, a_2^2 a_3 a_5 + \\ + 8\, a_2^3 a_6)/(2a_2)^9 \tag{13e}$$

From eqs. (7), (8a), (11) and (13) the Lagrangian is

$$L(q,\dot q) = a_o + \sum_{m=1}^{\infty} (-i\, b_m(q)\dot q + B_m(q))(\dot q - a_1(q))^m$$

$$B_m(q) = \sum_{n=1}^{m} i^n\, a_n(q) \sum_{m=\sum_{j=1}^{n} m_j} \prod_{j=1}^{n} b_{m_j}(q) \tag{14}$$

and substituted in eq. (2) it gives the solution of the master equation. The Euler-Lagrange equation for $L(q,\dot q)$ gives the evolution equation of $q(t)$.

While the above general approach completely solves the problem of finding the Lagrangian it is clearly very cumber-some if the Kramers-Moyal series does not sum to a definite analytic function. On the otherhand if the series is truncated after a few terms then the Lagrangian in eq. (14) can be exhibited in closed form. This is the case of the Fokker-Planck equation for non-zero drift and diffusion coefficients $T_1(q)$ and $T_2(q)$ respectively. From eqs. (1) and (13) we find that all $b_m(q)=0$ except $b_1(q)$. For the Lagrangian one gets

$$L(q,\dot q) = \frac{1}{4a_2}(\dot q + a_1)^2 - a_o \tag{15}$$

where

$$a_o(q) = \frac{V_o''}{V_o} T_2 + \frac{V_o'}{V_o}(2T_2' + T_1) + (T_2'' + T_1') \tag{16a}$$

$$a_1(q) = 2\frac{V_o'}{V_o} T_2 + (2T_2' + T_1) \tag{16b}$$

$$a_2(q) = T_2 \tag{16c}$$

and for the evolution equation we have

$$\ddot{q}(t) = \frac{a_2'}{2a_2} (\dot{q}^2 - a_1^2) + (a_1 a_1' - 2a_2 a_o') \tag{17}$$

Eq. (15) reproduces the result of Dekker[6] and Graham[2] for constant diffusion coefficient ($T_2(q) = 1/2$)

$$L(q, \dot{q}) = \frac{1}{2} (\dot{q} + T_1(q))^2 - \frac{1}{2} T_1'(q) \tag{15'}$$

if the integration path in eq. (2) is deformed to pass through a critical point $q = q_c$ of the autonomous system

$$\begin{aligned} \dot{q} &= v \\ \dot{v} &= \frac{a_2'}{2a_2} (v^2 - a_1^2) + (a_1 a_1' - 2a_2 a_o') \end{aligned} \tag{18}$$

so as to maximise the path integral. For this it is necessary to recall that $V_o(q)$ satisfies the differential equation

$$a_2(q) V_o''(q) + a_1(q) V_o'(q) + a_o(q) V_o(q) = 0. \tag{19}$$

Hence for q near q_c

$$\frac{V_o''(q)}{V_o(q)} = - (T_2'' + T')/2\, T_2 \tag{20}$$

It is useful to always multiply the rhs of eq. (7) by an energy parameter ω. Doing this one finds for linearized processes that

$$L(q, \dot{q}) = \frac{1}{4\omega\sigma} (\dot{q} + \omega q)^2 - \omega^2 \left(1 - \frac{1}{2\sigma}\right) \tag{21}$$

where σ is the variance of the equilibrium Gaussian.

REFERENCES. -

(1) - N. Hashitsume; Proc. of the Inter. Conf. on Theoretical Physics (Kyoto 1958) p. 495.

(2) - R. Graham; Springer Tracts in Modern Physics Vol. 66 p. 1.

(3) - R. Graham; in "Fluctuations, Instabilities and Phase Transitions" ed. T. Riste (New York 1975) p. 215.

(4) - L. Onsager and S. Machlup; Phys. Rev. 91, 1505 (1953), 91, 1512 (1953).

(5) - N. G. Van Kampen, Fundamental Probelms in Statistical Mechanics; ed. E. G. D. Cohen (Amsterdam 1962) p. 173.

(6) - H. Dekker; Phys. Letters 65A, 382 (1978) and references therein.

(7) - R. Kubo, K. Matsuo and K. Kitahara; Journ.of Statistical Phys. 9, 51 (1973).

(8) - H. Behnke and F. Sommer; Theorie der Funktionen einer Komplexen Veränderlichen (Springer Berlin 1955).