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E. Etim and C. Basili: ON THE STOCHASTIC PROPERTIES OF THE THERMODYNAMIC HAMILTONIAN.

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ABSTRACT. -

If the generalised momentum in the Hamiltonian equations is considered as arapidly varying stochastic function of time then a solution of the master equation is most easily obtained by applying the central limit theorem in much the same way as one does with the Langevin equation.

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Given the Kramers-Moyal series

$$\mathcal{M}(q, \frac{\partial}{\partial q}) = \sum_{n=1}^{\infty} (\alpha \frac{\partial}{\partial q})^n T_n(q) \tag{1}$$

one can derive the reversible equation of motion for q(t) from the Hamiltonian[1]

$$H(q,p) = i \sum_{n=0}^{\infty} a_n(q)(ip)^n$$

$$a_n(q) = \varphi_o^{-1}(q) \sum_{\ell=n}^{\infty} \binom{\ell}{n} (\alpha \frac{d}{dq})^{\ell-n} (T_\ell(q)\, \varphi_o(q)) \tag{2}$$

$$p = -\, i\alpha \frac{\partial}{\partial q}$$

$\varphi_o(q)$ is the lowest eigenfunction of $\mathcal{M}(q, \partial/\partial q)$. Since the deterministic equation for q is obtained by eliminating p, the question arises as to whether the same result cannot be achieved by means of an appropriate average in which $\langle p(t) \rangle$ vanishes or is at most $O(\alpha)$.

The Hamiltonian equations could then be regarded as stochastic equations, and it should be possible to obtain from them a solution of the master equation in much the same way as one does for the Fokker-Planck equation, starting from the Langevin equation. By repeated application of the Markof property the path integral solution

$$W(q,t) = \int \mathcal{D}(q) \exp\left(\int_0^t d\tau\, L(q(\tau), \dot{q}(\tau))\right) \tag{3}$$

where $L(q, \dot{q})$ is the Lagrangian associated with $H(q,p)$, will thus follow directly from the statistical properties of the Hamiltonian equations. This argument suggests an implicit equivalence between the stochastic differential equation for q(t) and the partial differential equation for its probability distribution. We consider this problem here not for the full Hamiltonian but for the following analog of a non-relativistic approximation[2]

$$H_2(q,p) = \sum_{n=0}^{\infty} a_n(q)(ip)^n \tag{4}$$

The Hamiltonian for linearised processes is of the from (4). In general eq. (4) can be transformed into a harmonic oscillator Hamiltonian[2]. It therefore describes Gaussian processes. We wish to show that from the point of view of the question posed in the beginning, the Gaussian approximation to eq. (3) is indeed most easily obtained by attributing stochastic properties to the generalised momentum in the equations[3]

$$\frac{\partial H_2(q,p)}{\partial p} = \dot{q} = -(a_1(q)+2a_2 ip) \tag{5a}$$

$$\frac{\partial H_2(q,p)}{\partial q} = -\dot{p} = i(a_0'(q)+a_1'(q)ip+a_2'(q)(ip)^2) \tag{5b}$$

and then applying to the integral of eq. (5a) the central limit theorem. This fact is not at all surprising from the point of view of quantum mechanics, for, from the definition of p in eq. (1), eqs. (5a) and (5b) are operator equations and p and q do not commute. Eqs. (5) are classical equations only in the sense of the Ehrenfest theorem.

We shall therefore assume that:

1) $p(t)$ is a rapidly varying function of time on a scale τ_0 small compared to that characteristic of variations of $q(t)$.
2) the mean and variance of the distribution $\Phi(u)$ of the velocity

$$u(\tau_0) = i \int_t^{t+\tau_0} d\tau \; p(\tau) \tag{6}$$

exist.

Eq. (5a) can be expressed in terms of $u(\tau_0)$ as

$$q(t)-x(t) = \sum_{k=0}^{N=t/\tau_o} 2a_2(k\tau_o)u(\tau_o) \tag{7}$$

where

$$\dot{x}(t) = -a_1(x) \tag{8}$$

describes the average motion of q(t) and we have written $a_2(t)$ for $a_2(q(t))$. On taking the average of both sides of eqs. (5) we have

$$\langle p(t) \rangle = 0 \tag{9a}$$

$$\langle p^2(t)\rangle = a_0'(x)/a_2'(x) \tag{9b}$$

If t is much greater than τ_o we can apply the central limit theorem[4] to eq. (7) to get

$$W(q,t) = (2\pi\alpha\sigma(t))^{-1/2} \exp(-\frac{(q(t)-x(t))^2}{2\alpha\sigma(t)}) \tag{10}$$

where

$$\sigma(t) = 4D \int_0^t a_2^2(\tau)\, d\tau \tag{11}$$

and $\sigma_0=D\tau_o$ is the variance[5] of $\Phi(u)$. The distribution $\Phi(u)$ need not be a Gaussian in order for (10) to hold. However if the distribution of p(t) is a Gaussian, (obtainable, say, by Fourier transforming W(q,t) as in quantum mechanics) then so too is $\Phi(u)$.

Eq. (11) can be integrated indirectly. First differentiate it to get

$$\dot{\sigma}(t) = 4D\, a_2^2(x) \tag{12}$$

The variance $\sigma(t)$ can also be calculated approximately from

$$2\alpha\sigma(t)= \int_{-\infty}^{+\infty} dq\; \varphi_o(q)\, \hat{q}^2(t)\, \varphi_o(q)-x^2 \tag{13}$$

where $\varphi_0(q)$ is the ground state of $H_2(q,p)$[2] and $\hat{q}(t)$ is an operator whose time derivative is given by eq. (5a). By expanding the coefficients $a_n(q)$ about q=x

$$a_n(q) = a_n(x) + a'_n(x)\,(q-x) + \frac{1}{2} a''_n\,(q-x)^2 + \ldots\ldots \tag{14}$$

one finds from eq. (13)

$$\dot{\sigma}(t) = -\,2a'_1(x)\sigma(t)+2(a_2(x)+xa'_2(x)) \tag{15}$$

On comparing this with eq. (12) we get

$$\sigma(t) = -\,\frac{1}{a'_2(x)}\,(2D\,a_2^2(x) - a(x)-xa'_2(x)) \tag{16}$$

In eq. (9a) the average value of p(t) is strictly zero as a consequence of eq. (8). This estimate can be improved. The change of variables[2]

$$\begin{aligned} i\omega^{1/2}P &= a_2^{1/2}\,(ip - \frac{a_1}{2a_2}) \\ \frac{1}{2}\,\omega^{1/2}Q &= (\frac{a_2^1}{4a_2} - a_o)^{1/2} \end{aligned} \tag{17}$$

in eq. (14) transforms the Hamiltonian into

$$H_2(Q,P) = i\,(\omega\,P^2 + \frac{\omega}{4}\,Q^2) \tag{18}$$

The generator of this transformation is of the form

$$F(q,P) = f_1(q)\,P + f_2(q) \tag{19}$$

where from the equations

$$\begin{aligned} \frac{\partial F(q,P)}{\partial q} &= p = (\frac{\omega}{a_2})^{1/2}\,P - i\,\frac{a_1}{2a_2} \\ \frac{\partial F(q,P)}{\partial P} &= Q = \frac{2}{\omega^{1/2}}\,(\frac{a_1^2}{4a_2} - a_o)^{1/2} \end{aligned} \tag{20}$$

the functions $f_1(q)$ and $f_2(q)$ are given by

$$\frac{df_1(q)}{dq} = (\frac{\omega}{a_2})^{1/2} = \frac{2}{\omega^{1/2}} \frac{d}{dq} (\frac{a_1^2}{4a_2} - a_o)^{1/2} \tag{21a}$$

$$\frac{df_2(q)}{dq} = - i \frac{a_1}{2a_2} \tag{21b}$$

On making use of eq. (21a) one finds that the equation of motion for Q(t) can be expressed in terms of q(t) as

$$\dot{q}(t) = - a_1(1-4a_o a_2)^{1/2} \tag{22}$$

Comparing this with (5a) gives

$$i \langle p(t) \rangle \simeq a_o(x)\, a_1(x) \tag{23}$$

since $a_o(x)$ is $0(\alpha)$.

The extension of the above considerations to the full Hamiltonian in eq. (2) is not straightforward. However the effect of the term in $(ip)^3$ in eq. (2) is easily incorporated into $H_2(q, p)$. In fact solving for p from the equation

$$\frac{\partial H_3(q, p)}{\partial p} = \dot{q} = - (a_1 + 2a_2 ip + 3a_3 (ip)^2) \tag{24}$$

and either by explanding the square root or by the integral method of ref. (1) one finds

$$- ip = \frac{(\dot{q} + a_1)}{2a_2}\ {}_2F_1 (\frac{1}{2}, 1; 2; - \frac{3a_3(\dot{q} + a_1)}{a_2^2}) \tag{25}$$

If eq. (23) is used to substitute for $\dot{q} + a_1$ inside the hypergeometric function one sees from eq. (5a) and the equality

$$-ip = \frac{(\dot{q}+a_1)}{2a_2}\; {}_2F_1\left(\frac{1}{2};\, 1;\, 2,\, -\frac{6a_o a_1 a_3}{a_2}\right) =$$

$$= \frac{(\dot{q}+a_1)}{a_2\left(1+\left(1+\frac{6a_o a_1 a_3}{a_2}\right)^{1/2}\right)} \qquad (26)$$

that the effect of the term in $a_3(q)$ is to renormalise the coefficient $a_2(q)$, and consequently the variance $\sigma(t)$ on account of eq. (11).

REFERENCES.

1) E.Etim and C.Basili, Phys. Letters A (to be published); Frascati preprint LNF-78/19(P) (1978).
2) E. Etim and C. Basili, Frascati preprint LNF-78/26(P) (1978). (Submitted to Phys. Letters A).
   Since the Hamiltonian H(q, p) contains the unknown function $\varphi_o(q)$ it is suggested in this reference to determine it by successive approximations.
3) Dots denote derivatives with respect to time and primes derivatives with respect to q.
4) H. Cramér; The Elements of Probability Theory, John Wiley Inc. New York (1966) p. 114.
5) Our use of this term is not strictly correct because from eq. (10) $\alpha\sigma(t)$ is the variance.