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E. Etim and C. Basili : ON THE CONTACT TRANSFORMATIONS OF NON-EQUILIBRIUM THERMODYNAMIC HAMILTONIAN.

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ABSTRACT. -

The Hamiltonian governing the time evolution of stationary fluctuation states contains both dissipative and irreversible effects. We use a contact transformation to disentangle them.

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For a system with no critical or unstable equilibria the solution of the master equation

$$\alpha \frac{\partial W(q,t)}{\partial t} = \mathscr{M}(q, \frac{\partial}{\partial q}) W(q,t)$$

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

in the limit $\alpha \longrightarrow 0$ is well approximated by a Gaussian[1, 2]. The path integral representation of such a solution

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

is nothing more then a repeated application of the Markof property. Although not unique the Lagrangian in eq. (2) is unambiguous. On account of eq. (1) it should contain not only the effects of dissipation but also irreversibility, making it unnecessary to postulate special path independent weighting factors in eq. (2) to account for the latter[3]. In a previous letter[4] we have discussed the construction of the Lagrangian directly from the operator $\mathscr{M}(q, \partial/\partial q)$. We wish here to show how by means of a contact transformation the Lagrangian so constructed can be separated into its dissipative and irreversible parts. This exercise will confirm that eq. (2) has to be evaluated as it stands.

Let $W_o(q) = \varphi_o^2(q)$ be the ground state in the eigenfunction equation

$$\mathscr{M}(q, \frac{\partial}{\partial q}) W_n(q) = -\lambda_n W_n(q) \tag{3}$$

We define the Hamiltonian associated with (1) by

$$H(q,p) = i\, \varphi_o^{-1}(q) \mathscr{M}(q, \partial/\partial q) \varphi_o(q)$$

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

where

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

$$p = -i\alpha \frac{\partial}{\partial q} \tag{5}$$

By inverting the series[5]

$$\frac{\partial H(q,p)}{\partial p} = \dot{q} = -\sum_{n=1}^{\infty} n\,a_n(q)(ip)^{n-1} \tag{6}$$

to solve for p in terms of q and $\dot{q}$ the Lagrangian is computed from eq. (4) by means of the Legendre transformation. If H(q,p) is not a simple analytic function of p the Lagrangian obtained in this way is extremely complicated and has necessarily to be approximated. The approximation we adopt here is suggested by the formal analogy between eq. (4) and the expansion in powers of the momentum of the relativistc Hamiltonian of a particle in an electromagnetic field in 2-space-time dimensions[6]

$$H_{EM}(q,p) = e\,\phi(q) + \sum_{n=0}^{\infty} a_n^{EM}(q)(ip)^n = e\phi(q) + (m^2c^4 + (p - \frac{e}{c}A(q))^2)^{1/2}$$

$$a_n^{EM}(q) = -\frac{1}{2} \sum_{\ell=n}^{\infty} \binom{\ell}{n} \left(-i\,\frac{e\,A(q)}{c}\right)^{\ell-n} \left(\frac{\ell!}{(\ell-1)(\frac{\ell}{2})!\,(m\,c^2)^{\ell-1}}\right) \tag{7}$$

In the limit $\alpha \longrightarrow 0$ we get the analog of the non-relativistic approximation of (7) if powers of p greater than the second are neglected in eq. (4). The resulting Hamiltonian is

$$H(q,p) = i \sum_{n=0}^{2} a_n(q)\,(ip)^n \tag{8}$$

with corresponding Lagrangian

$$L(q,\dot{q}) = -i(p\frac{\partial H}{\partial p} - H) = \frac{(\dot{q}+a_1)^2}{4\,a_2} - a_o \tag{9}$$

Since the $a_n(q)$ in eq. (5) contain the unknown function $\varphi_o(q)$ the Hamiltonian H(q,p) is to be determined by successive approximations: one starts by setting $\varphi_o(q) = \varphi_o^{(o)}(q)$ = constant in eq. (15), computes $H^{(o)}(q,p)$ and then determines $\varphi_o^{(1)}(q)$ from

$$H^{(o)}(q,p)\ \varphi_o^{(1)}(q) = 0 \tag{10}$$

and so on. The first step in this iteration already gives the a_n (q) as power series in α and will be sufficient for most purposes.

Now the change of variables

$$\begin{aligned} i\omega^{1/2} P &= a_2^{1/2} \ (ip - \frac{a_1}{2\,a_2}) \\ \frac{1}{2}\ \omega^{1/2} Q &= (\frac{a_1^2}{4\,a_2} - a_o)^{1/2} \end{aligned} \tag{11}$$

in eq. (8), where ω is a constant, transforms the Hamiltonian into

$$\hat{H}(Q,P) = i\,(\omega P^2 + \frac{\omega}{4}\ Q^2) \tag{12}$$

with corresponding Lagrangian

$$\begin{aligned} \hat{L}\,(Q,\ \dot{Q}\,) &= -\,i\,(P\dot{Q} - \hat{H}\,(Q,P)) \\ &= \frac{1}{4\,\omega}\ (\dot{Q} + \omega^2\ Q^2) \end{aligned} \tag{13}$$

The generator of the transformation in eq. (11) is[7]

$$F(q,P) = f_1(q)\ P + f_2(q) \tag{14}$$

where, from the equations

$$\frac{\partial F(q,P)}{\partial q} = p = (\frac{\omega}{a_2})^{1/2}\, P - i\,\frac{a_1}{2a_2} \tag{15a}$$

$$\frac{\partial F(q,P)}{\partial P} = Q = \frac{2}{\omega^{1/2}}\ (\frac{a_1^2}{4a_2} - a_o)^{1/2} \tag{15b}$$

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

$$\frac{df_1(q)}{dq} = (\frac{\omega}{a_2})^{1/2} = \frac{2}{\omega^{1/2}} \frac{d}{dq} (\frac{a_1^2}{4a_2} - a_o)^{1/2} \tag{16a}$$

$$\frac{df_2(q)}{dq} = - i \frac{a_1}{2a_2} \tag{16b}$$

The difference between the Lagrangians in eqs. (9) and (13) is, on making use of eq. (16a)

$$L(q, \dot{q}) - \hat{L}(Q, \dot{Q}) = - \dot{q} \frac{a_1}{2a_2} = \frac{dS(q)}{dt} \tag{17}$$

where

$$S(q) = S_0 - \frac{1}{2} \int_0^q du \frac{a_1(u)}{a_2(u)} \tag{18}$$

The equation of motion for Q(t)

$$\ddot{Q} = \omega^2 Q \tag{19}$$

is, again on making use of eq. (16a), equivalent to

$$\dot{q} = \pm a_1 (1 - 4a_2 a_o)^{1/2} \tag{20}$$

Since $a_2(q)$ is positive, eq. (20) with the negative sign gives upon substitution in eq. (17)

$$\frac{dS}{dt} = \frac{a_1^2}{2a_2} (1 - 4 a_2 a_o)^{1/2} > 0 \tag{21}$$

For linearized processes $a_o(q) = 0$, $a_1(q) = q$, $a_2(q) = \sigma$ hence

$$\frac{dS}{dt} = \frac{q^2}{2\sigma} \tag{22}$$

coincides with the entropy production. Eq. (17) therefore achieves the separation of $L(q, \dot{q})$ into its dissipative and irreversible parts. That $L(q, \dot{q})$ contains both these effects follows from the fact that the operator $\mathscr{M}(q, \partial/\partial q)$ in the master equation also does. Irreversibility should not be put in by hand in the path integral representation[3].

Finally note that if $a_o(q) \neq 0$ then eq. (20) and the equation of motion

$$\ddot{q} = \frac{a_2'}{2a_2}(\dot{q}^2 - a_1^2) + a_1 a_1' - 2a_2 a_o' \tag{23}$$

obtained by varying $L(q, \dot{q})$ yield the relation

$$a_o(q) = \frac{\text{const.}}{1-a_1^2(q)} = \alpha \frac{c}{1-a_1^2(q)} + 0(\alpha^2) \tag{24}$$

Substituting the first terms of eq. (5) in (24) and integrating we get

$$T_1^3(q) - 3T_1(q) - 3cq = 0(\alpha) \tag{25}$$

If $c^2q^2 > 2/3$, eq. (25) has one real solution

$$\begin{aligned} T_1(q) &= \left(-\frac{3}{2}cq + \left(\frac{9}{4}c^2q^2 - 1\right)^{1/2}\right)^{1/3} + \\ &+ \left(-\frac{3}{2}cq - \left(\frac{9}{4}c^2q^2 - 1\right)^{1/2}\right)^{1/3} \equiv T_+(q) + T_-(q) \end{aligned} \tag{26}$$

while if $c^2q^2 < 2/3$ all solutions are real

$$\begin{aligned} T_1^{(1)}(q) &= (T_+ + T_-) \simeq \sqrt{3} - \frac{1}{2}cq + 0(q^2) \\ T_1^{(2)}(q) &= -\frac{1}{2}(T_+ + T_-) + i\frac{3}{2}(T_+ - T_-) \simeq -\sqrt{3} - \frac{1}{2}cq + 0(q^2) \\ T_1^{(3)}(q) &= -\frac{1}{2}(T_+ + T_-) - i\frac{\sqrt{3}}{2}(T_+ - T_-) \simeq cq + 0(q^2) \end{aligned} \tag{27}$$

For small q, $T_1^{(3)}(q)$ gives the linearized approximation. The other solutions have no zeroes in $c^2q^2 < 2/3$ to satisfy the equilibrium condition

$$\ddot{q} \simeq a_1 a_1' = 0 \tag{28}$$

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(5) We use dots to denote differentiation with respect to t and primes for differentiation with respect to q.

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