A VARIATIONAL PRINCIPLE FOR THE AVERAGE VALUE AND THE DISPERSION OF AN OPERATOR ; APPLICATION TO MEAN FIELD THEORY

H. FLOCARD

Division de Physique Théorique+, Institut de Physique Nucléaire, F-91406 ORSAY

This communication was prepared in collaboration with R. Balian, P. Bonche and M. Vénéroni.

I- INTRODUCTION

In a recent letter[1)] Balian and Vénéroni proposed a variational principle for the measure of observables in evolving systems. In this section we list some properties which, in our opinion, should be satisfied by any such principle.

a) A measurement involves two objects : an operator which corresponds to the observable of interest, and a density matrix which describes the system under consideration. An operator and a density matrix appear therefore as logical ingredients for a variational principle, the goal of which is the description of a measurement.

b) In an actual experiment the system is prepared at some initial time t_0, i.e. its density matrix D is known at that time. The trial density matrix $\mathcal{D}(t)$ which is to enter the variational principle should therefore satisfy

$$\mathcal{D}(t_0) = D \ .$$

The actual density matrix $\mathcal{D}(t)$ evolves then according to the Von-Neumann equation up to some time $t_1 > t_0$, at which the measurement is performed by using a specific apparatus which is described by an operator A . If we note $\mathcal{A}(t)$ the trial operator at any time we must have

$$\mathcal{A}(t_1) = A \ .$$

In other words, any variation on $\mathcal{A}$ and $\mathcal{D}$ consistent with the nature of a measurement at t_1, on a system prepared at t_0, should satisfy

$$\delta \mathcal{D}\big|_{t_0} = 0 \qquad ; \qquad \delta \mathcal{A}\big|_{t_1} = 0 \quad . \tag{1}$$

c) Although the usefulness of the principle will show up mainly when approximations will be introduced, it should also provide the exact equations of motion for the most general variation of the trial operator and density, $\mathcal{A}$ and $\mathcal{D}$.

d) It appears also desirable that the stationary "action" should possess the physical meaning of the quantity for which the principle has been built, i.e. the result of the measurement. This requirement that the action should have physical significance is for example not satisfied by the canonical Schrödinger variational principle for the wave-function $|\Psi\rangle$

$$\delta I_s = 0 \;;\; I_s = \int_{t_0}^{t_1} dt \,\langle \Psi | \frac{d}{dt} + i H | \Psi \rangle \quad .$$

Indeed when solutions of this variational principle are inserted into the action I_s, this quantity does not acquire any particular significance : it vanishes for the actual solution.

II- A VARIATIONAL PRINCIPLE FOR THE AVERAGE VALUE OF AN OPERATOR

From the considerations of the preceding section, Balian and Vénéroni were led to propose the following principle

$$\delta I = 0 \quad ; \quad I = \mathrm{Tr}\mathcal{A}\mathcal{D}\big|_{t_1} - \int_{t_0}^{t_1} dt\, \mathrm{Tr}\, \mathcal{A}\left(\frac{d\mathcal{D}}{dt} + i[H,\mathcal{D}]\right) \tag{2}$$

Although, several mean field approximations can be derived from this variational principle, the trial density $\mathcal{D}$ is not constrained to be normalized. This feature turns out to be cumbersome for the application we are interested in (evaluation of dispersions). This is why we start anew with the following slightly modified principle.

$$\delta I_a = 0 \;;\; I_a = \frac{\mathrm{Tr}\mathcal{A}\mathcal{D}}{\mathrm{Tr}\mathcal{D}}\bigg|_{t_1} - \int_{t_0}^{t_1} dt\, \mathrm{Tr}\, \mathcal{A}\left(\frac{d}{dt}\frac{\mathcal{D}}{\mathrm{Tr}\mathcal{D}} + i\left[H, \frac{\mathcal{D}}{\mathrm{Tr}\mathcal{D}}\right]\right)$$
$$\delta \mathcal{A}\big|_{t_1} = 0 \qquad ; \qquad \delta \mathcal{D}\big|_{t_0} = 0 \tag{3}$$

In both definition (2) and (3) of an action, H is the hamiltonian and Tr stands for the trace in the Fock space in which the operators $\mathcal{A}(t)$ and $\mathcal{D}(t)$ act.

For any variational subspaces the variations with respect to $\mathcal{A}$ and $\mathcal{D}$ lead to the equations

$$\left\{\begin{array}{l} \mathrm{Tr}\ \delta\mathcal{A}\left(\frac{d\tilde{\mathcal{D}}}{dt}+i\,[H,\tilde{\mathcal{D}}]\right)=0 \quad ; \quad \tilde{\mathcal{D}}\equiv\frac{\mathcal{D}}{\mathrm{Tr}\mathcal{D}} \\ \mathrm{Tr}\,\frac{\delta\mathcal{D}}{\mathrm{Tr}\mathcal{D}}\left\{\frac{d\mathcal{A}}{dt}+i\,[H,\mathcal{A}]-\mathrm{Tr}\tilde{\mathcal{D}}\left(\frac{d\mathcal{A}}{dt}+i[H,\mathcal{A}]\right)\right\} \end{array}\right. \quad * \tag{4.a}$$

These equations can be equivalently written as

$$\left\{\begin{array}{l} \delta_{\mathcal{A}}\,\mathrm{Tr}\ \mathcal{A}\left(\frac{d\tilde{\mathcal{D}}}{dt}+i\,[H,\tilde{\mathcal{D}}]\right)=0 \\ \delta_{\mathcal{D}}\,\mathrm{Tr}\ \tilde{\mathcal{D}}\left(\frac{d\mathcal{A}}{dt}+i\,[H,\mathcal{A}]\right)=0 \end{array}\right. \tag{4.b}$$

where $\delta_{\mathcal{A}}$ and $\delta_{\mathcal{D}}$ stand for the variations with respect to the parameters which define $\mathcal{A}$ and $\mathcal{D}$ in the particular subspaces considered. For an arbitrary choice of these subspaces the existence of solutions to the equations (4) is not guaranteed. It will have to be checked for every particular choice.

If the equations (4) have a solution, then along a trajectory

$$\delta\mathcal{A}=\frac{d\mathcal{A}}{dt}\,\delta t \qquad\qquad \delta\mathcal{D}=\frac{d\mathcal{D}}{dt}\,\delta t$$

are certainly allowed variations. Inserting them into (4) and subtracting the equations, we find that the quantity

$$\mathcal{E}_a=-i\,\mathrm{Tr}\,\mathcal{A}\,[H,\tilde{\mathcal{D}}] \tag{5}$$

is conserved along any trajectory. $\mathcal{E}_a$ is the invariant associated with the time translational invariance of the principle (3), and as such can be called a pseudo-energy.

Let us now find a condition on the variational space for $\mathcal{A}$ which will <u>ensure the property d) presented in the first section, namely that the stationary</u>

* Note the distinct appearance of $\mathcal{D}$ and $\tilde{\mathcal{D}}$ in this second equation.

value of the action I_α is equal to the average value of the operator A at time t_1 (in the restricted space chosen for the density matrix). If a variation $\delta\mathcal{A}$ proportional to $\mathcal{A}$ is possible, equation (4.a) tells us that any solution of the equation of motion satisfies

$$\mathrm{Tr}\,\mathcal{A}\left(\frac{d\tilde{\mathcal{D}}}{dt}+i[H,\tilde{\mathcal{D}}]\right)=0 \tag{6}$$

and the action (3) is indeed equal to the average value of A :

$$I_\alpha = \mathrm{Tr}\,\mathcal{A}\tilde{\mathcal{D}}\big|_{t_1} = \mathrm{Tr}\,A\tilde{\mathcal{D}}\big|_{t_1} \quad . \tag{7}$$

From now on,we assume that the above condition ($\delta\mathcal{A}\propto\mathcal{A}$ allowed) will be satisfied by the variational space for the operator $\mathcal{A}(t)$.

We have now to check the point c) of the introduction by considering the most general variation for the operator $\mathcal{A}$ and the density matrix $\mathcal{D}$. We find first an equation for the normalized density

$$\frac{d\tilde{\mathcal{D}}}{dt}+i[H,\tilde{\mathcal{D}}]=0 \quad . \tag{8}$$

This is the Von Neumann equation for $\tilde{\mathcal{D}}$. We note that due to the invariance of the action I_α under the gauge transformation

$$\mathcal{D}(t) \longrightarrow (\exp f(t)).\,\mathcal{D}(t) \quad ; \quad f(t_0)=0 \tag{9}$$

we have no information on the evolution of the norm of $\mathcal{D}$. This however does not affect the value of the action. The second equation, once we take eq.(6) into account, writes

$$\frac{d\tilde{\mathcal{A}}}{dt}+i[H,\tilde{\mathcal{A}}]=0 \tag{10}$$

with

$$\tilde{\mathcal{A}} = \mathcal{A} - \mathrm{Tr}\,\mathcal{A}\mathcal{D} \quad . \tag{11}$$

In other words, up to an unspecified constant, the time evolution of $\mathcal{A}$ follows the Schrödinger equation *. This undeterminacy on $\mathcal{A}$, which has no effect whatsoever on the result of the measurement since $\mathcal{A}$ is fully specified at the time of interest t_1 ($\mathcal{A}(t_1) = A$), results also from the invariance of the action under a gauge transformation :

$$\mathcal{A}(t) \rightarrow \mathcal{A}(t) + g(t) \;\; ; \;\; g(t_1) = 0 \tag{12}$$

The simplest way to remove the uncertainty on $\mathcal{A}$ is to impose

$$\frac{d}{dt} \operatorname{Tr} \mathcal{A} \tilde{\mathcal{D}} = 0$$

which implies that the time evolution of $\mathcal{A}$ is governed by the equation

$$\frac{d\mathcal{A}}{dt} + i [H, \mathcal{A}] = 0$$

We postpone to section IV the application of eq.(4) to mean field theory and turn now to the extension of the variational principle to the case of the dispersion of an operator.

III- EXTENSION OF THE PRINCIPLE TO MEASURE THE DISPERSION OF AN OPERATOR

Given variational subspaces for $\mathcal{A}$ and $\mathcal{D}$, we have determined an optimal answer to the problem of measuring, at time t_1, the expectation value $\langle A \rangle$ of the operator A and we know that

$$I_a = \langle A \rangle \tag{13}$$

In a next step we would like to use the same variational spaces to obtain an optimal value for the dispersion Δ of the operator A (at the same time t_1) around its average value $\langle A \rangle$. To do so, we consider the action

---

* Note that $\mathcal{A}(t)$ cannot be identified with an operator in the Schrödinger representation (which is a constant). Rather if we denote it : $\mathcal{A}(t_1, t)$, it obeys the Heisenberg equation with respect to t_1 and the Schrödinger eq.(10) with respect to t .

$$I_{\mathcal{A}} = \mathrm{Tr}\, \mathcal{A}^2 \tilde{\mathcal{D}} \Big|_{t_1} - \int_{t_0}^{t_1} dt\, \mathrm{Tr} \left\{ \mathcal{A}^2 \left(\frac{d\tilde{\mathcal{D}}}{dt} + i \,[H, \tilde{\mathcal{D}}] \right) - \lambda \mathcal{A} \tilde{\mathcal{D}} \right\} \tag{14.a}$$

which is to be extremized with respect to $\mathcal{A}(t)$ and $\mathcal{D}(t)$ subject to the conditions

$$\delta \mathcal{A} \Big|_{t_1} = 0 \qquad \mathcal{A}(t_1) = A - \langle A \rangle$$
$$\delta \mathcal{D} \Big|_{t_0} = 0 \tag{14.b}$$

and where the Lagrange parameter λ is adjusted so as to ensure

$$\mathrm{Tr}\, \mathcal{A} \tilde{\mathcal{D}} = 0 \tag{15}$$

Due to the conditions (14.b), (15) the quantity $\mathrm{Tr}\, \mathcal{A}^2 \tilde{\mathcal{D}} \big|_{t_1}$, which, as we shall see , is the stationary value of the action $I_{\mathcal{A}}$, turns out to be the dispersion of A measured at time t_1 (within the restricted supspace adopted for the variation of $\mathcal{D}$).

$$\mathrm{Tr}\, \mathcal{A}^2 \mathcal{D} \Big|_{t_1} \equiv \Delta = \mathrm{Tr}\, A^2 \tilde{\mathcal{D}} - (\mathrm{Tr}\, A \tilde{\mathcal{D}})^2 \Big|_{t_1} \tag{16}$$

The principles (3) and (14) which have the same structure appear thus as the first two steps towards an utilization of the variational spaces for $\mathcal{A}$ and $\mathcal{D}$ in order to achieve an optimal knowledge of the results of the interaction of the system with the operator A . Indeed generalizations of (14) to higher moments of A are simple.

Let us now derive the equations of motion associated with the action (14). One finds

$$\mathrm{Tr} \left\{ \delta(\mathcal{A}^2) \left(\frac{d\tilde{\mathcal{D}}}{dt} + i\,[H, \tilde{\mathcal{D}}] \right) - \lambda\, \delta\mathcal{A}\, \tilde{\mathcal{D}} \right\} = 0 \;; \quad \delta(\mathcal{A}^2) = \delta\mathcal{A}.\mathcal{A} + \mathcal{A}.\delta\mathcal{A}$$
$$\mathrm{Tr}\; \delta\tilde{\mathcal{D}} \left(\frac{d\mathcal{A}^2}{dt} + i\,[H, \mathcal{A}^2] + \lambda \mathcal{A} \right) = 0 \;; \quad \tilde{\mathcal{D}} = \mathcal{D} / \mathrm{Tr}\, \mathcal{D} \tag{17}$$

An other useful formulation is

$$\delta_{\mathcal{A}} \operatorname{Tr} \left\{ \mathcal{A}^2 \left(\frac{d\tilde{\mathcal{D}}}{dt} + i\,[H,\tilde{\mathcal{D}}] \right) - \lambda \mathcal{A} \tilde{\mathcal{D}} \right\} = 0 \tag{18}$$

$$\delta_{\mathcal{D}} \operatorname{Tr} \tilde{\mathcal{D}} \left(\frac{d\mathcal{A}^2}{dt} + i\,[H,\mathcal{A}^2] + \lambda \mathcal{A} \right) = 0$$

As in the preceding section we find a constant of motion $\mathcal{E}_d$ associated with the time translational invariance of the action (14).

$$\mathcal{E}_d = -i \operatorname{Tr} \mathcal{A}^2 [H,\tilde{\mathcal{D}}] \tag{19}$$

Similarly the restriction to subspaces for $\mathcal{A}$ which allow variations $\delta\mathcal{A}$ proportional to $\mathcal{A}$ ensures the desired result that the action I_d verifies

$$I_d = \operatorname{Tr} \mathcal{A}^2 \tilde{\mathcal{D}} \Big|_{t_1} = \Delta \tag{20}$$

The most general variation for $\mathcal{A}$ and $\mathcal{D}$ leads to the equations.

$$\left\{ \mathcal{A} ,\ \frac{d\tilde{\mathcal{D}}}{dt} + i\,[H,\tilde{\mathcal{D}}] \right\}_+ = \lambda \tilde{\mathcal{D}}$$

$$\left\{ \mathcal{A} ,\ \frac{d\mathcal{A}}{dt} + i\,[H,\mathcal{A}] \right\}_+ = -\lambda \mathcal{A} + \frac{d}{dt} \operatorname{Tr} \mathcal{A}^2 \tilde{\mathcal{D}} \tag{21}$$

where the curly brackets stand for anticommutators. The exact equations of motion

$$\frac{d\tilde{\mathcal{D}}}{dt} + i\,[H,\tilde{\mathcal{D}}] = 0 \quad ; \quad \frac{d\mathcal{A}}{dt} + i\,[H,\mathcal{A}] = 0 \quad ; \quad \lambda = 0 \tag{22}$$

are evidently solutions of equations(21). By considering the matrix equations obtained by writing eq.(21) in the basis which diagonalizes $\mathcal{A}(t)$ one sees that most of the matrix elements are identical to those obtained from the exact equations (22). In other words, it is only in some subspaces (in particular the kernel of $\mathcal{A}$) that spurious solutions may arise.

IV- APPLICATION TO THE MEASURE OF A ONE-BODY OPERATOR

Let us now derive the equations for a particular choice of the variational subspaces. We shall restrict $\mathcal{A}(t)$ (and thus A) to be a one-body operator of the type

$$\mathcal{A} = \frac{a}{2} + \sum_{ij} c_i^+ B_{ij} c_j \tag{23}$$

where the set of operators $\{c_i^+\}$, i = 1..N generates the Fock space, the number a and the matrix elements B_{ij} being $\mathbb{C}$-numbers* . For $\mathcal{D}$ we adopt the variational space of uncorrelated density matrices :

$$\mathcal{D} = p \cdot \exp \sum_{ij} c_i^+ R_{ij} c_j \tag{24}$$

where again p and R_{ij} are $\mathbb{C}$ -numbers. These uncorrelated density operators are in one to one correspondance with the set of numbers formed by the partition function Z plus the one-body density matrix $\{\rho_{ij}\}$ defined by

$$\begin{aligned} Z &= \mathrm{Tr}\,\mathcal{D} \\ \rho_{ij} &= \mathrm{Tr}\, c_j^+ c_i \mathcal{D} / \mathrm{Tr}\,\mathcal{D} \equiv \frac{1}{2}(\delta_{ij} + M_{ij}) \end{aligned} \tag{25}$$

(We introduce the NxN matrix M which allows a simpler form for the equations of motion).

A) Equations of motion for the average value

We first consider the equations associated with the action I_a . To derive the explicit form of the equations of motion (4.b) we must evaluate the quantities $\mathrm{Tr}\,\mathcal{A}\frac{d\tilde{\mathcal{D}}}{dt}$, $\mathrm{Tr}\,\tilde{\mathcal{D}}\frac{d\mathcal{A}}{dt}$ and $\mathrm{Tr}\,\mathcal{A}[H,\tilde{\mathcal{D}}]$. This can be done easily by means of the Wick theorem which applies for density matrices of the form (24). One finds

*In ref.(1) similar equations were derived (although not explicitly written) for the slightly more general case of operators which do not commute with the particle number operator.

$$2\,\mathrm{Tr}\,\mathcal{A}\tilde{\mathcal{D}} = a + \mathrm{tr}\,B(1+M)$$

$$2\,\mathrm{Tr}\,\mathcal{A}\frac{d\tilde{\mathcal{D}}}{dt} = \mathrm{tr}\,B\dot{M} \tag{26}$$

$$2\,\mathrm{Tr}\,\tilde{\mathcal{D}}\frac{d\mathcal{A}}{dt} = \dot{a} + \mathrm{tr}\,\dot{B}(1+M)$$

In the above equations the notation tr indicates a trace in the one-body space labelled by the index i = 1 ... N whereas Tr denotes a trace in the Fock-space ; the dots indicate a time derivative. For the Hamiltonian H of the many fermions system , we choose

$$H = \sum_{ij} t_{ij}\, c_i^+ c_j + \frac{1}{4}\sum_{ijkl} V_{ijkl}\, c_i^+ c_j^+ c_l c_k \tag{27}$$

with

$$V_{ijkl} = -V_{jikl} = -V_{ijlk} \tag{28}$$

Then the pseudo-energy (5) writes :

$$\mathcal{E}_a = -i\,\mathrm{Tr}\,\mathcal{A}[H,\tilde{\mathcal{D}}] = -\frac{i}{2}\,\mathrm{tr}\,B[W,M] \tag{29}$$

where the Hartree-Fock hamiltonian W is given by

$$W_{ij} = t_{ij} + \frac{1}{2}\sum_{kl} V_{iljk}\,(1+M)_{kl}$$

It is convenient to introduce the notation

$$\sum_{kl} V_{iljk}\, C_{kl} = {}^{\mathrm{tr}}V^{C}_{ij}$$

so that the NxN matrix W takes the form

$$W = t + \frac{1}{2}\,{}^{\mathrm{tr}}V^{(1+M)} \tag{30}$$

Let us now perform the variations implied by equation (4.b), where $\delta\mathcal{A}$ stands for δa and δB_{ij} whereas $\delta\mathcal{D}$ stands for δz and δM_{ij}. The variations with respect to a and z lead to two identities 0 = 0. This results from the two gauge invariances already noted ((9), (12)) which are still present in the restricted variational spaces used in this section. We recall that the undeterminacy associated with these gauge transformations does not affect the final result. The variations with respect to B_{ij} and M_{ij} give the two matrix equations

$$\dot{M} + i\,[W, M] = 0 \tag{31.a}$$

$$\dot{B} + i\,[W, B] + i\,T = 0 \tag{31.b}$$

where we introduced the additional mean field T

$$T = \frac{1}{2}\,\mathrm{tr}_2\, V^{[B,M]} \tag{32}$$

Eq.(31.a) is the usual T.D.H.F. equation. It is completely decoupled from the time evolution of B. This is the "happy accident" noted in ref.(1) : the T.D.H.F evolution in the space of uncorrelated density matrices is optimal whatever one-body operator is to be measured at the final time t_1. On the other hand, the time evolution of B, described by eq.(31.b) is coupled to that of M through the action of the two mean fields W and T. It is not however necessary to solve eq.(31.b) since, the operator $\mathcal{A}(t_1) = A$ being known at the final time, its expectation value can be computed once the T.D.H.F. equation has been solved. As a last remark we note that the T.D.H.F. equations (31) are not restricted by the condition $M^2 = 1$ (or $\rho^2 = \rho$) which states that the density matrix corresponds to a pure state with a determinantal wave function.

B) <u>Equations of motion for the dispersion</u>

We shall now derive the explicit form of the equations (18) associated with the action I_{cl}. To do so, we must evaluate the quantities $\mathrm{Tr}\,\mathcal{A}^2\frac{d\tilde{\mathcal{D}}}{dt}$, $\mathrm{Tr}\,\tilde{\mathcal{D}}\frac{d\mathcal{A}^2}{dt}$ and $\mathrm{Tr}\,\mathcal{A}^2[H,\tilde{\mathcal{D}}]$. Using again the Wick theorem one finds

$$
\begin{aligned}
2\,\mathrm{Tr}\,\mathcal{A}\tilde{\mathcal{D}} &= a + \mathrm{tr}\,B(1+M) \equiv 2\bar{A} \\
4\,\mathrm{Tr}\,\mathcal{A}^2\tilde{\mathcal{D}} &= 4\bar{A}^2 + \mathrm{tr}\; B^2 - BMBM \\
2\,\mathrm{Tr}\,\mathcal{A}^2\frac{d\tilde{\mathcal{D}}}{dt} &= 2\bar{A}\,\mathrm{tr}\,B\dot{M} - \mathrm{tr}\,BMB\dot{M} \\
2\,\mathrm{Tr}\,\tilde{\mathcal{D}}\frac{d\mathcal{A}^2}{dt} &= 2\bar{A}\,(\dot{a} + \mathrm{tr}\,\dot{B}(1+M)) + \mathrm{tr}\,\dot{B}(B - MBM) \\
2\,\mathrm{Tr}\,\mathcal{A}^2[H,\tilde{\mathcal{D}}] &= -\,\mathrm{tr}\;([W,B]+T)(B-MBM) - 2\bar{A}\;\mathrm{tr}([W,B]M)
\end{aligned}
\qquad (33)
$$

In constrast with I_a, the action I_d is not invariant under the gauge transformation (12). Indeed shifting $\mathcal{A}^2$ by a constant will in general destroy the property of being the square of an operator. The practical implication is that the variation (18) with respect to a does not lead to an identity 0 = 0 (as does the variation with respect to Z). The variation with a provides a scalar equation which can be used to determine the Lagrange parameter λ . After some tedious but straightforward algebra, one ends up with the equations of motion, which write more conveniently in terms of two matrices X and Y measuring the deviations from the T.D.H.F. equations (31)

$$
\begin{aligned}
X &= \dot{M} + i\,[W,M] \\
Y &= \dot{B} + i\,([W,B]+T)
\end{aligned}
\qquad (34)
$$

In turn the matrices X and Y are obtained in terms of M and B by solving the following matrix equations

$$
\begin{aligned}
MBX + XBM &= i\,([S,M] - T + MTM) \\
BMY + YMB &= i\,([S,B] - U)
\end{aligned}
\qquad (35)
$$

where two new mean fields

$$
S = \frac{1}{2}\,{}^{\mathrm{tr}}\mathcal{V}^{\,B-MBM} \;;\quad U = \frac{1}{2}\,{}^{\mathrm{tr}}\mathcal{V}^{\,(BM)^2-(MB)^2} \qquad (36)
$$

have been introduced. From the knowledge of X and Y , we can evolve M and B by equation (34) and proceed further in time. In contrast with eq.(31), eqs.(34-35) describe a fully coupled motion of M and B , which makes the solution more difficult. In addition we recall that the operator B is not known at the initial time t_0 . An iterative process should thus be used (guessing some trial initial value $B(t_0)$) in order to ensure that $B(t_1)$ is indeed the operator chosen at the final time. The variation with respect to a along with the constraint $\mathrm{Tr}\, \mathcal{A}\tilde{\mathcal{D}} = 0$ provide us with two decoupled equations which give the time evolution of the Lagrange parameter λ and the operator constant a , once equations (34-35) have been solved

$$\begin{aligned} \lambda &= \mathrm{tr}\, BX \\ a &= -\mathrm{tr}\, B(1+M) \end{aligned} \qquad (37)$$

V- CONCLUSION

We propose a variational principle which can be used to extract successively the optimal average value and dispersion associated with the measure of a given operator at a final time t_1 on a system whose density matrix is known at some initial time t_0 . For the most general variations the exact equations of motion are recovered. In addition, the stationary values of the actions are equal to the quantities of interest, namely the average value and the dispersion measured in the variational space of the trial density matrices. We have derived the equations for the case of one-body operators and uncorrelated density matrices and showed how the time-dependent Hartree-Fock equations should be modified in order to evaluate a dispersion. Application to the Lipkin model is in progress.

Ref.(1) R. BALIAN, M. VENERONI, Phys. Rev. Let. 47(1981) 1353.

NOTE : Page 1355, 1st Col umn, 3nd Paragraph, the sentence "the best choice for $\mathcal{D}(t)$ does not depend ...", should be replaced by "the best choice for $\mathcal{D}(t)$ does depend ...".