A variational determination of multi-time correlation functions

R. Balian

PHYSIQUE THEORIQUE
SACLAY
CEA/DSM

T93/017

A variational determination of multi-time correlation functions

R. Balian
CEA/Saclay, Service de Physique Théorique[a]
F-91191 Gif-sur-Yvette Cedex, FRANCE

Statistical Description of Transport in Plasma, Astro- and Nuclear Physics
Les Houches, France
2-11 Février 1993
MISGUICH J., PELLETIER G., SCHUCK P. (eds.) *Nova, 1993*

[a] Unité associée CNRS/SPM/URA 2306

A variational determination of multi-time correlation functions

R. Balian
CEA/Saclay, Service de Physique Théorique[a]
F-91191 Gif-sur-Yvette Cedex, FRANCE

1 Statement of the problem

The purpose of this course is to present the general features of a work recently achieved with Marcel Vénéroni [1]. Part of the methods and results were already published in previous articles [2], but a synthesis has now been made, and a coherent though flexible scheme for evaluating correlations has emerged. Explicit calculations, proofs, details and references can be found in [1,2], and we shall thus restrict ourselves to the underlying ideas.

The general problems which we have in mind, and which are of relevance for the various topics of this workshop, are formally the following ones. Suppose the state $D(t_o)$ of a system of interacting particles is given at some initial time t_o. We consider some set of physical quantities Q_j, which are probabilistic but vary in time according to a known law, and we wish to evaluate their expectation values and their time-correlations.

This question covers many physical situations. For *classical statistical mechanics*, $D(t_o)$ is the initial density in phase, the Q_j are some functions of the positions and momenta of the particles; they are random due to the uncertainties contained in the initial condition $D(t_o)$, and evolve according to the Hamilton equations. For instance, in plasma physics, the expectation value of Q_j may represent either the density at some point (in which case j labels this point) or one of its Fourier components (in which case j labels a wave number); we can ask about density correlations either at different times or more simply at equal times. In cosmology, we are interested in correlations between the positions of galaxies in order to describe the large scale structure of the Universe.

For *quantum problems*, $D(t_o)$ is the density operator which describes the initial state. In the special case of a pure initial state, it reduces to the projection operator onto this state; in zero-temperature field theory, this can be the projection onto the vacuum. The quantities Q_j are some set of operators which represent the observables of interest in the Schrödinger picture and which will evolve in the Heisenberg picture. For instance, in the theory of nuclear *heavy ion collisions,* the state $D(t_o)$ represents the projectile and the target in their ground state, boosted towards each other. If we wish to describe statistically the sizes of the outgoing fragments, we can take as observables Q_j the operators which describe the numbers of nucleons lying in some or other region of space. Energy correlations can be obtained similarly. For studying correlations in the final state, we should take all the times t equal in the operators $Q_j^H(t, t_o)$ in the Heisenberg picture; taking different times provides information on time-delayed correlations. In the same

[a] Unité associée CNRS/SPM/URA 2306

problem, we may also be interested for theoretical purposes in the expectation values and correlations of single-particle (s.p.) observables.

The formalism will cover *equilibrium* questions, in which case $D(t_0)$ is a Boltzmann-Gibbs distribution, as well as *non-equilibrium* questions. For definiteness and for the sake of generality, we shall focus on quantum many-body problems, governed by a Hamiltonian H, and shall illustrate the approach by an example which leads to an elaborate extension of the mean-field theory for interacting fermions. Application to finite temperature field theories may also be considered [3,4,5].

We shall write the *initial state* as

$$D(t_0) \equiv e^{-\beta \mathcal{H}}, \tag{1.1}$$

since usually $\ln D(t_0)$ is a simpler operator than $D(t_0)$ itself. The form (1.1) ensures positivity; for grand canonical equilibrium, $\mathcal{H}$ equals $H - \mu N$ where μ is the chemical potential and β is the inverse temperature. More generally, the use of the maximum entropy criterion leads naturally to expressions of the type (1.1) where $\mathcal{H}$ is a linear combination of the (in general simple) observables on which information is available. Pure states can be recovered from (1.1) in the limit as $\beta \longrightarrow \infty$ for a suitable choice of $\mathcal{H}$. In collision theory we take $\mathcal{H} = H_1 + H_2 - v.p$ where H_1 and H_2 are the Hamiltonians of the two incoming fragments, p is their relative momentum operator and v their relative velocity. We shall find it convenient not to normalize $D(t_0)$ (see).

Denoting by Q_j the *observables of interest* in the Schrödinger picture, their counterpart in the Heisenberg picture is given by the Heisenberg equation

$$\frac{dQ_j^H(t', t_0)}{dt'} = -i\left[Q_j^H(t', t_0), H\right], \tag{1.2}$$

we assume that H and Q_j do not depend explicitly on time. The boundary condition

$$Q_j^H(t_0, t_0) = Q_j \tag{1.3}$$

is imposed at the initial time t_0. We have let $\hbar = 1$, and should replace commutators by Poisson brackets for classical problems.

We wish to evaluate quantities of the following types.

(i) *Expectation values* at a time t .

$$\langle Q_j(t)\rangle \equiv \mathbf{Tr}\ D(t_0)\, Q_j^H(t, t_0) / \mathbf{Tr}\ D(t_0), \tag{1.4}$$

which do not depend on t for equilibrium problems, where $D(t_0)$ commutes with H.

(ii) *Thermodynamic quantities*. In particular, for a grand canonical equilibrium where $\mathcal{H} = H - \mu N$, the grand potential is given as function of the temperature $T = \beta^{-1}$ and the chemical potential μ by

$$\begin{aligned} A(T,\mu) &= -\frac{1}{\beta} \ln \mathbf{Tr}\ D(t_0) \\ &= \langle H - \mu N\rangle - TS \end{aligned} \tag{1.5}$$

The entropy S, free energy, internal energy, pressure, follow by taking partial derivatives of A.

(iii) *Causal two-time correlation functions:*

$$\begin{aligned} C_{jk}(t', t'') \equiv\ & \mathbf{Tr}\ T\ D(t_0)\, Q_j^H(t', t_0)\, Q_k^H(t'', t_0) / \mathbf{Tr}\ D(t_0) \\ & - \langle Q_j(t')\rangle \langle Q_k(t'')\rangle, \end{aligned} \tag{1.6}$$

where the time-ordering T-product acts on t' and t''.

(iv) *Ordinary correlations*, obtained from (1.6) by letting $t'' = t'$. If we are not interested in the dynamics, correlations between the Q_j in the state $D(t_0)$ are found for $t'' = t' = t_0$.

(v) *Fluctuations*, obtained from (1.6) by letting $t'' = t'$ and $k = j$.

(vi) *Cross-sections*, obtained from (1.4) by taking for Q_j a projector and by letting $t_0 \longrightarrow -\infty$, $t \longrightarrow +\infty$.

(vii) *Causal multi-time functions* or *higher order correlations*, which are cumulants of several operators, similar to (1.6), possibly with equal times.

(viii) *Response functions:*

$$\chi_{jk}\left(t',t''\right) = -i\theta\left(t'-t''\right) \boldsymbol{Tr}\left[Q_j^H\left(t',t_o\right),Q_k^H\left(t'',t_o\right)\right] D\left(t_o\right) / \boldsymbol{Tr}\ D\left(t_o\right), \tag{1.7}$$

which describe the first-order correction

$$\delta\left\langle Q_j\left(t'\right)\right\rangle \sim \int_{t_o}^{\infty} \boldsymbol{dt''} \sum_k \chi_{jk}\left(t',t''\right)\zeta_k\left(t''\right) \tag{1.8}$$

induced on the expectation value $\left\langle Q_j\left(t'\right)\right\rangle$ by a small time-dependent perturbation $\sum_k \zeta_k(t) Q_k(t)$ added to the Hamiltonian H at any time $t > t_o$.

Both the initial state (1.1) and the Heisenberg operators (1.2) are usually extremely complicated, due to correlations and interactions between the elementary particles which constitute the system. For weak interactions, perturbative approaches are efficient. For stronger interactions, variational approaches of the mean-field type often provide satisfactory results for bulk quantities like (1.5) or s.p. expectation values like (1.4), but are obviously ill-suited for correlations. Indeed, in a variational method such as the Hartree-Fock method, one looks for the minimum of some functional, which is the best approximation for the grand potential (or for the ground state energy). However, using subsequently the state thus determined for evaluating correlations is not a variational procedure, since this method optimizes only the grand potential. We are thus not surprised that it yields trivial results. Instead, our purpose is to build up a systematic variational formalism where the very functional that we make stationary directly provides the required correlations. Our strategy relies on merging a few general ideas which we present in sects. 2 to 5.

2 Generating functional

The first of these ideas is a well-known basic technique of field theory. There, in order to build the Green's functions, one introduces sources and one defines a functional of these sources, analogous to a partition function. Expanding it in powers of the sources then generates the Green's functions.

Likewise, we introduce time-dependent *sources* $\xi_j(t)$ associated with each of the observables Q_j, and define the generating functional for these observables by

$$\varphi\{\xi\} \equiv \boldsymbol{ln}\ \boldsymbol{Tr}\ D\left(t_o\right) A\left(t_o\right), \tag{2.1}$$

$$A\left(t_o\right) \equiv T\ \boldsymbol{exp}\ i \int_{t_o}^{\infty} \boldsymbol{dt'} \sum_j \xi_j\left(t'\right) Q_j^H\left(t',t_o\right). \tag{2.2}$$

In classical statistical mechanics, $D\left(t_o\right)$ and $A\left(t_o\right)$ are functions of a point in the many-body phase space, and $\boldsymbol{Tr}$ is meant for an integration over this point.

The expansion of φ in powers of the sources ξ reads

$$\begin{aligned}\varphi\{\xi\} &= \boldsymbol{ln}\ \boldsymbol{Tr}\ D\left(t_o\right) + i \sum_j \int_{t_o}^{\infty} \boldsymbol{dt'}\xi_j\left(t'\right)\left\langle Q_j\left(t'\right)\right\rangle \\ &- \frac{\boldsymbol{1}}{\boldsymbol{2}} \int_{t_o}^{\infty} \boldsymbol{dt'dt''} \sum_{jk} \xi_j\left(t'\right)\xi_k\left(t''\right) C_{jk}\left(t',t''\right) + \ldots .\end{aligned} \tag{2.3}$$

It thus generates to first order the expectation values (1.4), to second order the causal two-time correlation functions (1.6), and more generally the full sequence of multi-time causal functions. Just as for the second *characteristic function* in probability theory, the inclusion of a logarithm in the definition (2.1) accounts for the substractions which enter the definition of cumulants. The lack of normalization of $D\left(t_o\right)$ affects only the zeroth-order term in (2.3), which for equilibrium statistical mechanics yields the thermodynamic potential (1.5).

Our purpose will thus be to evaluate approximately φ, a single quantity which encompasses the various questions that we are asking. The difficulty lies in the intricate form of both the initial state $D\left(t_{\mathrm{o}}\right)$, assumed to be given in the form (1.1) which is most often not easily manageable, and the operator $A\left(t_{\mathrm{o}}\right)$. In the definition (2.2) of the latter, the time-dependent operators $Q_j^H\left(t', t_{\mathrm{o}}\right)$ are complicated, even though usually the Schrödinger operators Q_j are not; moreover they do not commute at different times t'. We wish to determine φ variationally, and to this aim we shall need beforehand to characterize the objects $D\left(t_{\mathrm{o}}\right)$ and $A\left(t_{\mathrm{o}}\right)$ by simple equations. This will be the object of the next two sections.

3 Backward Heisenberg equation

In spite of the complexity of the operator $A\left(t_{\mathrm{o}}\right)$, we shall show that it can be generated by a formally simple differential equation, provided we replace the initial time t_{o} in its definition (2.2) by a time t which will run from $\rightharpoondown\infty$ back to t_{o}. We thus introduce the operator

$$A\leftharpoonup t\leftharpoondown \equiv T\ \boldsymbol{exp}\ i\int_t^{\infty} \boldsymbol{dt'} \sum_j \xi_j\left(t'\right) Q_j^H\left(t', t\right), \qquad \leftharpoonup 3.1 \leftharpoondown$$

which still depends on the sources $\xi_j\left(t'\right)$ for $t' > t$ in a complicated fashion, but depends moreover on the time t. Let us focus on this dependence.

We are led to regard the *Heisenberg operators* $Q_j^H\left(t', t\right)$ as functions of *two times*, the usual running time t', and also the reference time t at which they coincide with the Schrödinger operators as in (1.3). However, instead of being fixed at the initial time t_{o} as usual, this reference time is now regarded as a second running time. We take advantage of this fact and write a differential equation for $Q_j^H\left(t', t\right)$ in terms of t. By using the formal explicit expression

$$Q_j^H\left(t', t\right) \,/\, U^{\dagger}\left(t', t\right) Q_j U\left(t', t\right) \qquad \leftharpoonup 3.2 \leftharpoondown$$

in terms of the evolution operator $U\left(t', t\right)$ from t to t', and the properties of U, we readily find

$$\frac{\boldsymbol{d}Q_j^H\left(t', t\right)}{\boldsymbol{dt}} \,/\, i\left[Q_j^H\left(t', t\right), H\right]. \qquad \leftharpoonup 3.3 \leftharpoondown$$

The differential equation (3.3) should for each t' be solved together with the final boundary condition

$$Q_j^H\left(t', t'\right) \,/\, Q_j, \qquad \leftharpoonup 3.4 \leftharpoondown$$

and hence the time t should be considered as *running backwards.*

We call (3.3) the backward Heisenberg equation ♭2a♮. It plays the same role in quantum mechanics as the backward Kolmogorov equation does in the theory of Markov processes, where the forward Kolmogorov equation (the equivalent of the standard Heisenberg equation) is identified with the Fokker-Planck equation. Both the forward equation (1.2) and the backward one (3.3), together with the associated boundary condition (1.3) or (3.4), have (3.2) as solution. Nevertheless the backward equation is the only useful one here, since the time t' is integrated over in the definition (3.1) of $A\leftharpoonup t\leftharpoondown$. Let us note moreover that the backward Heisenberg equation, in spite of its somewhat weird feature of involving a change in the reference time t rather than in the observation time t', is more general than the ordinary one. Indeed, if the Hamiltonian H or the Schrödinger operator Q_j *depend explicitly on time*, the Heisenberg equation (1.2) is replaced by

$$\frac{\boldsymbol{d}Q_j^H\left(t', t\right)}{\boldsymbol{dt'}} \,/\, -i\left[Q_j^H\left(t', t\right), U^{\dagger}\left(t', t\right) H\left(t'\right) U\left(t', t\right)\right] \rightharpoondown U^{\dagger}\left(t', t\right) \frac{\boldsymbol{d}Q_j}{\boldsymbol{dt'}} U\left(t', t\right). \qquad \leftharpoonup 3.5 \leftharpoondown$$

It is no longer a closed equation for Q_j^H, as its solution requires the determination of $U(t', t)$. In contrast, the backward equation (3.3) remains unchanged, within the replacement of H by $H(t)$, while the time dependence of Q_j is accounted for by the boundary condition (3.4). This backward equation is thus a better means than the forward one for generating the operators Q_j^H in the Heisenberg picture. Note also that the classical counterpart of (1.2) is the Hamilton equation (written with a Poisson bracket), supplemented by an initial condition in terms of a random point in phase space; on the other hand, the classical counterpart of (3.3) is obtained by shifting infinitesimally the initial time t for a similar final boundary condition.

In the definition (3.1) of $A(t)$, we have not only changed the reference time of the Heisenberg picture into t, but also cut-off the sources at the times t' earlier than t. The derivative of $A(t)$ with respect to t thus involves a term arising from (3.3) and another one from the lower integration bound, namely

$$\frac{dA(t)}{dt} = i[A(t), H] - iA(t)\sum_j \xi_j(t) Q_j. \qquad (3.6)$$

Moreover, the integrand in (3.1) vanishes as $t \longrightarrow \infty$, whence

$$A(+\infty) = 1. \qquad (3.7)$$

The operator $A(t_0)$ is therefore obtained by solving the differential equation (3.6) backward in time, from $t = +\infty$ where we have the boundary condition (3.7), down to $t = t_0$. The equation (3.6) is formally simple. It *disentangles the various dependences of* $A(t)$, as it accounts for the *evolution* through H and for the *sources* through its last term. The ordering of operators in this term reflects the occurrence of the T-product in the definition of $A(t)$, for an anti-T-product, it would be reversed. It is remarkable that all the complications of $A(t_0)$, and in particular its functional dependence on the sources, come out only from the integration of (3.6).

4 A simple equation for the initial state

Since $\mathcal{H}$ in (1.1) is usually a simple operator, typically a sum of one- and two-particle operators, the complications of $D(t_0)$ arise from taking its exponential. We can, here also, generate this exponential by replacing β by a variable u going from 0 to β and taking the derivative with respect to u. This yields the *Bloch equation*

$$\frac{d}{du} e^{-u\mathcal{H}} = -\mathcal{H} e^{-u\mathcal{H}}. \qquad (4.1)$$

In order to stress an analogy with the equation (3.6) for $A(t)$, we introduce the complex time $t \equiv t_0 + i(\beta - u)$ and define

$$D(t) \equiv e^{-u\mathcal{H}} = e^{-i\mathcal{H}(t - t_0 - i\beta)}. \qquad (4.2)$$

The initial state $D(t_0)$ is then characterized as being the solution of the differential equation

$$\frac{dD(t)}{dt} = -i\mathcal{H} D(t), \qquad (4.3)$$

with the boundary condition

$$D(t_0 + i\beta) = 1. \qquad (4.4)$$

Here t runs from $t_0 + i\beta$ to t_0.

For the sake of symmetry, we introduce, as is usual in quantum statistical mechanics [3], an $\boldsymbol{L}$-shaped contour in the *complex plane of times* (fig. 1), oriented from $t_0 + i\beta$ to t_0 then to $+\infty$. The forward equation (4.3) for D and the backward equation (3.6) for A meet at t_0, where we want to calculate the generating functional φ through (2.1).

Figure 1 . The complex t-plane.

1

5 General method for constructing variational expressions

Our last step consists in replacing the set of equations (2.1), (3.6) and (4.3), which together with the boundary conditions (3.7) and (4.4) determine the quantity of interest φ, by a variational principle. To achieve this aim, we shall resort to a general method [2b,6] which produces systematically variational principles for problems of the following type:

Find the value

$$e^{\varphi} \equiv f\{X\} \tag{5.1}$$

taken by a function $f\{\mathcal{X}\}$ of some set of variables $\mathcal{X}_m$ at a point $\{\mathcal{X}_m\} / \{X_m\}$ which is characterized by a set of equations

$$g_n\{\mathcal{X}\} / 0. \tag{5.2}$$

In our case, the quantities X_m are the matrix elements of the two operators $A(t)$ at each time $t \geq t_0$ and $D(t)$ at each time $t_0 - i\beta < t \leq t_0$, and the single index m encompasses both the matrix indices and the (continuous) time. The equations (5.2) are the matrix elements at each time of the differential equations (3.6) and (4.3), and the quantity $\varphi / \ln f\{X\}$ is (2.1). Note that this quantity depends only on part of the variables X_m, since it involves only the time t_0.

We wish to construct a function (or a functional if m is a continous index) which will be equal to e^{φ} at its stationary point. In spite of the fact that the constraints (5.2) are in sufficient number to determine X_m, let us associate with them a set of Lagrangian multipliers $\mathcal{Y}_m$, and introduce the functional

$$\Phi\{\mathcal{X},\mathcal{Y}\} \equiv f\{\mathcal{X}\} - \sum_n \mathcal{Y}_n g_n\{\mathcal{X}\}. \tag{5.3}$$

(For a continuous index, the sum becomes an integral.) Infinitesimal variations of the variables $\mathcal{Y}_m$ and $\mathcal{X}_m$ produce changes

$$\delta\Phi / -\sum_n d\mathcal{Y}_n g_n\{\mathcal{X}\}, \tag{5.4}$$

$$\delta\Phi / \sum_m d\mathcal{X}_m \left[\frac{\partial f\{\mathcal{X}\}}{\partial \mathcal{X}_m} - \sum_n \mathcal{Y}_n \frac{\partial g_n\{\mathcal{X}\}}{\partial \mathcal{X}_m}\right], \tag{5.5}$$

respectively. If $\boldsymbol{\Phi}$ is stationary under unrestricted variations of the $\mathcal{Y}$'s, the vanishing of (5.4) is equivalent to (5.2). Hence the stationary value of the functional $\boldsymbol{\Phi}$ with respect to the multipliers $\mathcal{Y}$ is the required quantity (5.1). If moreover $\boldsymbol{\Phi}$ is stationary with respect to the $\mathcal{X}$'s, the vanishing of (5.5) determines in the space $\{\mathcal{X},\mathcal{Y}\}$ a saddle-point of (5.3) where $\boldsymbol{\Phi}$ equals e^{φ} (fig. 2).

Figure 2 . *A geometric interpretation of the general variational method.* The two axes symbolize the coordinates $\{\mathcal{X}\}$ and $\{\mathcal{Y}\}$, respectively. The altitude represents the value of $\Phi\{\mathcal{X},\mathcal{Y}\}$, the level lines of which have been drawn. When one sits near the saddle point, one approaches the searched quantity e^{φ} (the altitude of the saddle-point) within a second-order error. Using the stationarity of Φ with respect to $\{\mathcal{X}\}$ eliminates half of the variables, and forces one to remain on the dashed-dotted line $\mathcal{Y}(\mathcal{X})$. When Φ has a suitable curvature, $\Phi\{\mathcal{X},\mathcal{Y}(\mathcal{X})\}$ follows the thalweg and the region explored in the variational treatment lies below the saddle-point.
2

These remarks lead to a variational principle of practical interest. Let us assume that the equations (5.2) are too intricate to be solved, and/or the evaluation of (5.1) at the point X is not tractable. Nevertheless, let us choose a trial set for $\{\mathcal{X},\mathcal{Y}\}$, as wide as possible, such that we can evaluate explicitly (5.3). This will be feasible if $f\{\mathcal{X}\}$ and $g_n\{\mathcal{X}\}$ have a sufficiently simple form, which is the case for (2.1), (3.6) and (4.3). Writing then that the variations (5.4), (5.5) vanish within the restricted subset provides the stationary value of $\boldsymbol{\Phi}$ in this subset. If the latter is suitably chosen, we may expect the result to lie close to e^{φ}, because the surface $\boldsymbol{\Phi}\{\mathcal{X},\mathcal{Y}\}$ is *flat* near its saddle-point (fig. 2); the error in φ is of *second-order* with respect to the errors in $\{\mathcal{X},\mathcal{Y}\}$. Thus, doubling the set of variables, and characterizing the exact solution by simple equations, allows us to set up a *variational scheme especially designed for the evaluation of the quantity* (5.1).

The examples given in refs.[2,6] show that this general approach encompasses many of the known variational principles used in physics. In particular, not only a stationary, but a maximum functional can be obtained when it is possible to eliminate the variables $\mathcal{Y}$ by means of (5.5) (see fig. 2). Moreover, refs.[2b,5] show how the variational principle based on (5.3) can be used for stochastic evolutions, or how it can fruitfully be combined with perturbative methods.

Applying this general technique to our problem, we introduce trial time-dependent operators $\mathcal{A}(t)$ for $t \geq t_0$ and $\mathcal{D}(t)$ for $t_0 + i\beta < t \leq t_0$, which are the variables $\mathcal{X}$ of the general theory, and their associated multipliers $\mathcal{Y}$. For the sake of symmetry, we denote these as $\mathcal{D}(t)$ for $t > t_0$, which is associated with the constraint (3.6) characterizing $A(t)$, and $\mathcal{A}(t)$ for $t_0 + i\beta < t < t_0$, which is associated with the constraint (4.3) characterizing $D(t)$. The determination of the generating functional φ then amounts to the search for the stationary value e^{φ} of the functional

$$
\begin{aligned}
&\Phi\{\mathcal{D}(t), \mathcal{A}(t)\} = \mathrm{Tr}\, \mathcal{D}(t_0 + i0)\, \mathcal{A}(t_0 + 0) + \\
&+ \mathrm{Tr} \int_{t_0}^{\infty} dt\, \mathcal{D}(t) \left\{ \frac{d\mathcal{A}(t)}{dt} - i[\mathcal{A}(t), H] + i\mathcal{A}(t) \sum_j \xi_j(t) Q_j \right\} \\
&- \mathrm{Tr} \int_{t_0 + i\beta}^{t_0} dt\, \mathcal{A}(t) \left\{ \frac{d\mathcal{D}(t)}{dt} + i\mathcal{K}\mathcal{D}(t) \right\}.
\end{aligned}
\qquad (5.6)
$$

The trial quantities $\mathcal{A}(t)$ and $\mathcal{D}(t)$, defined along the contour of fig. 1, which stand either for $A(t)$ if $t > t_0$ and $D(t)$ if $t_0 + i\beta < t < t_0$ or for multipliers along the remaining parts of the contour, should satisfy the boundary conditions

$$
\mathcal{A}(+\infty) = 1, \qquad \mathcal{D}(t_0 + i\beta) = 1. \qquad (5.7)
$$

Among the stationarity conditions (5.4), (5.5), we get from the variations with respect to $\mathcal{D}(t_0 + i0)$ and $\mathcal{A}(t_0 + 0)$

$$
\mathcal{A}(t_0 + i0) = \mathcal{A}(t_0 + 0), \qquad \mathcal{D}(t_0 + i0) = \mathcal{D}(t_0 + 0), \qquad (5.8)
$$

this continuity property explains why we chose the same notations for the variables and the multipliers. The various data on which φ depends, namely the Hamiltonian H, the observables Q_j, the sources $\xi_j(t)$, and the logarithm $-\beta\mathcal{K}$ of the initial density operator, enter (5.6) explicitly in a simple fashion.

6 Application to interacting fermions

In ref.[1] we have determined approximately the one- and two-time functions for a system of interacting functions by using the above variational principle. We rely on the fact that (5.6) can be evaluated explicitly if $\mathcal{A}(t)$ and $\mathcal{D}(t)$ are restricted to the subspace of *exponentials of s.p. operators.* Our trial space for $\mathcal{D}(t)$ is thus the same as in usual mean-field theories. Nevertheless, we find non-trivial results because our variational principle is especially suited to the determination of correlations. In other words, the best generating functional φ obtained from this formalism is not the one which would naively be inferred from the independent-particle state and evolution of a standard mean-field theory. Indeed, the optimization of (5.6) leads to approximate states and evolutions which *depend on the sources* $\xi_j(t)$, in spite of the use of the same trial states as in usual mean-field theories; it is this dependence which, together with the doubling of variables, generates the rather elaborate results that we find for the two-time correlation functions.

Let us briefly describe these results. We consider a Hamiltonian of the form

$$
H \equiv \sum_{\alpha\beta} B_{\alpha\beta} c^{\dagger}_{\alpha} c_{\beta} + \frac{1}{4} \sum_{\alpha\beta,\gamma\delta} \langle \alpha\beta \mid V \mid \gamma\delta \rangle c^{\dagger}_{\alpha} c^{\dagger}_{\beta} c_{\gamma} c_{\delta}, \qquad (6.1)
$$

and assume that $\mathcal{K}$ has also a similar form. For single-time expectation values (1.4), we find the same outcomes as in the usual mean-field theories. Namely, we have first to build the *static Hartree-Fock* density matrix ρ_0 associated with the s.p. state simulating $e^{-\beta\mathcal{K}}$. it is obtained by solving self-consistently the equation

$$
\rho_0 = \frac{1}{e^{\beta\mathcal{K}_0} + 1} \qquad (6.2)
$$

and the equation which expresses $\mathcal{K}_0$ as the s.p. reduction of $\mathcal{K}$ in terms of ρ_0. We then have to solve the *TDHF equation* associated with H,

$$
\frac{i d\rho^{(0)}(t)}{dt} = \left[W\left(\rho^{(0)}\right), \rho^{(0)} \right], \qquad (6.3)
$$

with $\rho^{\leftharpoonup 0 \leftharpoondown}(t_0) \;/\; \rho_0$ as an initial condition, where W is the s.p. reduction of H. (Classically (**6.3**) reduces to the Vlasov equation.) Finally, $\langle Q_j \leftharpoonup t \leftharpoondown \rangle$ is given in terms of $\rho^{\leftharpoonup 0 \leftharpoondown} \leftharpoonup t \leftharpoondown$ by means of *Wick's theorem.*

The results become more interesting when we expand φ up to second order in the sources so as to generate (**2.3**). The *best variational estimate* for (**1.6**) within our mean-field framework then involves *two RPA kernels,* $\mathcal{R}$ and $\not{\mathcal{R}}$. The first one, describing a time-dependence, is associated with $\rho^{\leftharpoonup 0 \leftharpoondown} \leftharpoonup t \leftharpoondown$ and H, according to

$$\sum_{\gamma\delta} \mathcal{R}_{\alpha\beta,\gamma\delta}\; x_{\delta\gamma} \equiv \left[W\left(\rho^{\leftharpoonup 0 \leftharpoondown}\right), x\right]_{\alpha\beta} \rightharpoondown \left[\boldsymbol{tr}_2 V_{12} x, \rho^{\leftharpoonup 0 \leftharpoondown} \sharp_{\alpha\beta}\right. . \qquad \leftharpoonup \mathbf{6.4} \leftharpoondown$$

Likewise the initial-state kernel $\not{\mathcal{R}}$ is associated with ρ_0 and $\not{H}$. Next, we have to introduce in the s.p. space a matrix $L_j\left(t', t\right)$ which is the image of Q^H and satisfies the equation (for $t < t' \leftharpoondown$

$$\frac{\boldsymbol{d}}{\boldsymbol{dt}} L_j\left(t', t\right) \;/\; i\; L_j\left(t', t\right) \mathcal{R} \leftharpoonup t \leftharpoondown, \qquad \leftharpoonup \mathbf{6.5} \leftharpoondown$$

with the final boundary condition $L_j\left(t', t'\right) \;/\; Q_j$. This *backward dual RPA* equation appears as the s.p. reduction of the backward Heisenberg equation, while the TDHF equation (**6.3**) appears as the s.p. reduction of the Liouville-von Neumann equation. The two-time correlation functions are then given by

$$C_{jk}\left(t', t''\right) \;/\; \tfrac{1}{2}\, \boldsymbol{tr}\; L_j\left(t', t_0\right) \leftharpoonup \boldsymbol{coth}\; \tfrac{1}{2}\beta \not{\mathcal{R}} \mp \mathbf{1} \leftharpoondown \left[L_k\left(t'', t_0\right), \rho_0\right], \quad t' \lessgtr t''. \qquad \leftharpoonup \mathbf{6.6} \leftharpoondown$$

For the linear responses (**1.7**), we get

$$\chi_{jk}\left(t', t''\right) \;/\; -i\; \theta\left(t', t''\right) \boldsymbol{tr}\left[L_j\left(t', t_0\right), L_k\left(t'', t_0\right)\right] \rho_0. \qquad \leftharpoonup \mathbf{6.7} \leftharpoondown$$

Thus, not only the HF and TDHF equations, but also the *RPA*, both *static* and *dynamic*, occur *variationally* here; this sheds a new light on this approximation. It should be noted that each of these building blocks has a specific use, the RPA beginning to play a rôle when we go from expectation values to correlations. However, in contrast to standard treatments, we get here a *backward* version of the RPA, with time flowing from t' to t_0. The two directions of time which enter our equations reflect the self-consistency of the scheme and the coupling between the approximations for $\mathcal{A} \leftharpoonup t \leftharpoondown$ and $\mathcal{D} \leftharpoonup t \leftharpoondown$.

Numerical calculations based on some preliminary results have been performed long ago for evaluating fluctuations in the number of nucleons of the outcoming fragments in heavy ion reactions [7]. They have shown that the present formalism brings in large corrections, which led to a better fit with experiment.

On the theoretical side, expressions like (**6.6**) and (**6.7**) constitute an important improvement on the outcome of ordinary mean-field theories. They obey many *consistency* requirements which are violated by the latter theories [1]. For instance, if the initial state is an equilibrium state, they depend only on the time difference $t' - t''$, as they should. They also satisfy the fluctuation-dissipation theorem, as well as properties arising from conservation or invariance laws.

In conclusion, let us stress again the generality of the approach. The use of a variational method based on the above ideas, and in particular of some or other variant of (**5.6**) should provide a flexible tool for dealing with problems from various branches of physics.

References

[1] [1] R. Balian and M. Vénéroni, submitted to Nucl. Phys. B.

[2] [2] R. Balian and M. Vénéroni, Ann. Phys. (N.Y.) (a) 164 (1985) 334; (b) 187 (1988) 29; (c) 195 (1989) 324; (d) 216 (1992) 351.

[3] [3] N.P. Landsman and Ch. van Weert, Phys. Reports 145 (1987) 141.

[4] [4] O. Eboli, R. Jackiw and S.-Y. Pi, Phys. Rev. D37 (1988) 3557.

[5] [5] A. Neveu, Nucl. Phys. B (Proc. Suppl.) 18B (1991) 242.

[6] [6] E. Gerjuoy, A.R.P. Rau and L. Spruch, Rev. Mod. Phys. 55 (1983) 725.

[7] [7] P. Bonche and H. Flocard, Nucl. Phys. A 437 (1985) 189; J.B. Marston and S.E. Koonin, Phys. Rev. Lett. 54 (1985) 1139; T. Troudet and D. Vautherin, Phys. Rev. C31 (1985) 278; M. Benarous, Thesis (Univ. Paris-Sud, Orsay, 1991).