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The functional formalism of classical statistical dynamics

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Abstract. A simple and general derivation of the functional formalism of classical statistical dynamics of Martin, Siggia and Rose is presented without the necessity of introducing non-commuting operators into the discussion. This is achieved by making use of functional integral representations of the correlation and response functions of the system. Some approximation procedures based on the functional integral representation are briefly discussed.

1. Introduction

The purpose of this paper is to provide a simple and general derivation of the functional formalism of classical statistical dynamics (to be referred to as the MSR formalism) which has been developed in the last three years. This is done by utilizing functional integral representations of the correlation and response functions of the system. The introduction of functional integrals in non-equilibrium statistical mechanics goes back to the work of Hosokawa (1967) and Rosen (1970), and the present paper provides an extension of their ideas.

In previous derivations of the MSR formalism (Martin *et al* 1973, Phythian 1975, 1976, Kawasaki 1974, Enz and Garrido 1976) an essential role has been played by certain operators which may roughly be described as creating excitations of the system. These are found to satisfy boson type commutation relations with the dynamical variables, together with an equation of motion consistent with such relations. The functional formalism is established by first showing that correlation and response functions for the system are given by averages of time-ordered products of such operators. A generating functional is then defined by means of a time-ordered exponential, and functional differential equations satisfied by this generating functional are derived. We shall refer to such equations as Schwinger equations since the analysis closely resembles that of Schwinger in the quantum theory of fields.

It has long been known that quantum mechanics can be formulated in terms of functional (path) integrals rather than operators and it is not surprising that the same is true of classical statistical dynamics. In fact this formulation already exists to some extent in the work of Hosokawa and Rosen on turbulence theory referred to above. The basic inadequacy of their work from our point of view is that it contains no discussion of response functions, however this deficiency can easily be removed as will be shown later. Functional integral representations of correlation functions have also been derived by Graham (1973) (see also Kubo *et al* 1973, Yahata 1974), for systems driven by white noise forces. While this work was being prepared a paper by Janssen (1976) appeared in which a representation of response functions was derived from Graham's results so obtaining a particular case of the results given here.

When a representation of both correlation and response functions has been found it is a simple matter to define a suitable generating functional in the form of a path integral from which the Schwinger equations may be derived. The restriction to Gaussian stirring forces or initial conditions which have been made previously can be relaxed without unduly complicating the discussion. It should be mentioned that, in unpublished work, Rose has also considered the non-Gaussian case using the operator method and reached similar conclusions to those reported here.

The functional integral representation is also useful in suggesting approximations which are difficult to formulate in any other way, and in conclusion we briefly describe some ideas along these lines.

2. The functional integral representation

We shall consider in detail a system described by a set of dynamical variables $\psi(\tau)=\{\psi_\alpha(\tau)\}$ which satisfy an equation of motion of the form

$$\dot{\psi}_\alpha(\tau)=f_\alpha(\tau)+\Lambda_\alpha(\psi(\tau),\tau). \tag{1}$$

Results will be stated later for a more general equation of motion. The quantities Λ_α are given non-random functions of the dynamical variables and time τ, while $f_\alpha(\tau)$ are random functions to be referred to as stirring forces. The probability distribution of these is given in terms of the characteristic functional defined as the expectation value

$$C[\phi]=\left\langle\exp\left(\mathrm{i}\int_{t_0}^{t}\mathrm{d}\tau\,\phi_\alpha(\tau)f_\alpha(\tau)\right)\right\rangle \tag{2}$$

which is defined for suitably well behaved test functions ϕ. We shall assume for simplicity that α ranges over the finite set of integers $1, 2, \ldots, M$, and a summation over repeated suffixes is implied. The system is regarded as being in a definite state at some initial time t_0, the dynamical variables having given values $\psi_\alpha^{(0)}$. We shall be interested in the situation during some finite but arbitrarily long time interval (t_0, t) and this is reflected in our definition of the characteristic functional. Without loss of generality the stirring forces can be taken as having zero mean. A situation in which there are random initial conditions can be described in the same way if the stirring forces are regarded as including random impulses acting at time t_0.

Our derivation of the functional integral makes use of the usual limiting procedure in which the time interval (t_0, t) is divided into N equal subintervals $(t_0, t_1), (t_1, t_2), \ldots$ of duration l, and the equation of motion is replaced by a difference equation. The most obvious difference equation to use is the one considered by Hosokawa and Rosen:

$$\frac{\psi_\alpha^{(n)}-\psi_\alpha^{(n-1)}}{l}=f_\alpha^{(n-1)}+\Lambda_\alpha(\psi^{(n-1)},t_{n-1})$$

which approximates the equation of motion to order l. Instead we shall consider the equation accurate to order l^2:

$$\frac{\psi_\alpha^{(n)}-\psi_\alpha^{(n-1)}}{l}=f_\alpha^{(n)}+\tfrac{1}{2}(\Lambda_\alpha(\psi^{(n)},t_n)+\Lambda_\alpha(\psi^{(n-1)},t_{n-1})) \tag{3}$$

where $f_\alpha^{(n)}$ denotes $f_\alpha(t_n^*)$ with $t_n^*=\tfrac{1}{2}(t_{n-1}+t_n)$. The equation (3) relates the two sets of variables $(f^{(1)}, \ldots, f^{(N)})$ and $(\psi^{(1)}, \ldots, \psi^{(N)})$. The corresponding probability density functions Q, P are related by the equation

$$P(\psi^{(1)}, \ldots, \psi^{(N)}) = JQ(f^{(1)}, \ldots, f^{(N)})$$

where J is the Jacobian determinant:

$$\det\left(\frac{\partial f_\alpha^{(n)}}{\partial \psi_\beta^{(m)}}\right) = \det\left(\frac{1}{l}\delta_{\alpha\beta}\delta_{nm} - \frac{1}{l}\delta_{\alpha\beta}\delta_{n-1,m} - \frac{1}{2}\Lambda_{\alpha,\beta}(\psi^{(n)}, t_n)\delta_{nm} - \frac{1}{2}\Lambda_{\alpha,\beta}(\psi^{(n-1)}, t_{n-1})\delta_{n-1,m}\right)$$

the comma notation denoting differentiation with respect to the variables ψ. The simplest way to evaluate this determinant is to write it in the form

$$\frac{1}{l^{NM}}\det(I+K)$$

where K is the matrix with elements

$$K_{\alpha\beta}^{(nm)} = -\delta_{\alpha\beta}\delta_{n-1,m} - \tfrac{1}{2}l\Lambda_{\alpha,\beta}(\psi^{(n)}, t_n)\delta_{nm} - \tfrac{1}{2}l\Lambda_{\alpha,\beta}(\psi^{(n-1)}, t_{n-1})\delta_{n-1,m}$$

and to use the identity

$$\det(I+K) = \exp \operatorname{Tr} \ln(I+K) = \exp \operatorname{Tr}(K - \tfrac{1}{2}K^2 + \ldots).$$

Since the elements of K above the diagonal $n = m$ are all zero it follows that $\operatorname{Tr} K^2$ is the sum of NM terms of order l^2, $\operatorname{Tr} K^3$ the sum of NM terms of order l^3 etc. In the limit as $l \to 0$ the only non-zero contribution comes from $\operatorname{Tr} K$ so we finally obtain

$$J = \frac{1}{l^{NM}} \exp\left(-\tfrac{1}{2}l \sum_{n=1}^{N} \Lambda_{\alpha,\alpha}(\psi^{(n)}, t_n)\right).$$

The probability density P is therefore given by

$$P(\psi^{(1)}, \ldots, \psi^{(N)}) = \frac{1}{l^{NM}} \exp\left(-\tfrac{1}{2}l \sum_{n=1}^{N} \Lambda_{\alpha,\alpha}(\psi^{(n)}, t_n)\right) Q(q^{(1)}, \ldots, q^{(N)})$$

with

$$q_\alpha^{(n)} = \frac{\psi_\alpha^{(n)} - \psi_\alpha^{(n-1)}}{l} - \frac{1}{2}(\Lambda_\alpha(\psi^{(n)}, t_n) + \Lambda_\alpha(\psi^{(n-1)}, t_{n-1})).$$

The probability density of the variables f is more conveniently expressed in terms of their joint characteristic function defined by

$$\mathscr{C}(\chi^{(1)}, \ldots, \chi^{(N)}) = \int df^{(1)} \ldots \int df^{(N)} Q(f^{(1)}, \ldots, f^{(N)}) \exp\left(\mathrm{i} \sum_{n=1}^{N} \chi_\alpha^{(n)} f_\alpha^{(n)}\right)$$

and using the inverse of this relationship we obtain

$$P(\psi^{(1)}, \ldots, \psi^{(N)}) = \frac{1}{(2\pi)^{NM}} \exp\left(-\tfrac{1}{2}l \sum_{n=1}^{N} \Lambda_{\alpha,\alpha}(\psi^{(n)}, t_n)\right) \times \int d\chi^{(1)} \ldots \int d\chi^{(N)} \mathscr{C}(l\chi^{(1)}, \ldots, l\chi^{(N)}) \exp\left(-\mathrm{i}l \sum_{n=1}^{N} \chi_\alpha^{(n)} q_\alpha^{(n)}\right). \quad (4)$$

It is apparent that in the limit as $l \to 0$

$$\mathscr{C}(l\chi^{(1)}, \ldots, l\chi^{(N)}) \to C[\chi]$$

where $\chi_\alpha^{(n)} = \chi_\alpha(t_n^*)$.

The mean value of a function F of the variables ψ may be written

$$\frac{\int d\psi^{(1)} \ldots \int d\psi^{(N)} \int d\chi^{(1)} \ldots \int d\chi^{(N)} F(\psi^{(1)}, \ldots, \psi^{(N)}) \mathscr{C}(l\chi^{(1)}, \ldots, l\chi^{(N)}) \times \exp(-\frac{1}{2}l \sum_n \Lambda_{\alpha,\alpha}(\psi^{(n)}, t_n) - il \sum_n \chi_\alpha^{(n)} q_\alpha^{(n)})}{\int d\psi^{(1)} \ldots \int d\psi^{(N)} \int d\chi^{(1)} \ldots \int d\chi^{(N)} \mathscr{C}(l\chi^{(1)}, \ldots, l\chi^{(N)}) \times \exp(-\frac{1}{2}l \sum_n \Lambda_{\alpha,\alpha}(\psi^{(n)}, t_n) - il \sum_n \chi_\alpha^{(n)} q_\alpha^{(n)})} \tag{5}$$

which in the limit gives the mean value of a functional $F[\psi]$ in the form

$$\langle F[\psi] \rangle = \frac{\int D[\psi] \int D[\chi] F[\psi] A[\psi, \chi]}{\int D[\psi] \int D[\chi] A[\psi, \chi]} \tag{6}$$

where the notation of Feynman and Hibbs (1965) has been used and A is given by

$$A[\psi, \chi] = C[\chi] \exp\left(-\frac{1}{2} \int_{t_0}^{t} d\tau\, \Lambda_{\alpha,\alpha}(\psi(\tau), \tau) - i \int_{t_0}^{t} d\tau\, \chi_\alpha(\tau) q_\alpha(\tau)\right) \tag{7}$$

with

$$q_\alpha(\tau) = \dot{\psi}_\alpha(\tau) - \Lambda_\alpha(\psi(\tau), \tau).$$

This is equivalent to the expressions derived by Hosokawa and Rosen as will be indicated later.

The ψ integration in (6) is to be taken over all trajectories in phase space consistent with the initial conditions. It is important to observe that in the expression (5) the limit of which defines the functional integral, the ψ and χ variables are considered at different times: the ψ at $t_1, \ldots, t_N$ and the χ at $t_1^*, \ldots, t_N^*$. In the same way an integral

$$\int D[\psi] \int D[\chi] F[\psi, \chi] A[\psi, \chi]$$

is defined in terms of a multiple integral in which F is replaced by a function of the values taken by ψ at $t_1, \ldots, t_N$ and by χ at $t_1^*, \ldots, t_N^*$. For example a functional of the form

$$\int_{t_0}^{t} d\tau\, g(\psi(\tau), \chi(\tau))$$

would be replaced by

$$\frac{1}{2}l \sum_{n=1}^{N} (g(\psi^{(n)}, \chi^{(n)}) + g(\psi^{(n-1)}, \chi^{(n)})$$

with $\psi^{(n)} = \psi(t_n)$ and $\chi^{(n)} = \chi(t_n^*)$. This definition of functional integrals has been discussed in detail by Katz (1965), and has the advantage of removing any ambiguity when the integrand involves ψ and χ evaluated at the same instant. It is equivalent to replacing $g(\psi(\tau), \chi(\tau))$ by

$$\frac{1}{2}(g(\psi(\tau), \chi(\tau - \epsilon)) + g(\psi(\tau), \chi(\tau + \epsilon)))$$

and taking the limit $\epsilon \to 0$ after the integration has been performed.

A particular case of (6) which will be needed later is the expression for the correlation function

$$U_{\alpha_1\ldots\alpha_n}(\tau_1,\ldots,\tau_n)=\langle\psi_{\alpha_1}(\tau_1)\ldots\psi_{\alpha_n}(\tau_n)\rangle=\frac{\int D[\psi]\int D[\chi]\psi_{\alpha_1}(\tau_1)\ldots\psi_{\alpha_n}(\tau_n)A[\psi,\chi]}{\int D[\psi]\int D[\chi]A[\psi,\chi]}.$$

We now examine the response of the system to a small perturbation of the stirring force. We consider a small non-random perturbation $e_\alpha(\tau)$ to be added to $f_\alpha(\tau)$ on the right-hand side of equation (1). The change in the expectation value of a functional F is then given by

$$\delta\langle F\rangle=\int d\tau\left\langle\frac{\delta F}{\delta f_\alpha(\tau)}\right\rangle e_\alpha(\tau)+\frac{1}{2!}\int d\tau\int d\tau'\left\langle\frac{\delta^2 F}{\delta f_\alpha(\tau)\delta f_\beta(\tau')}\right\rangle e_\alpha(\tau)e_\beta(\tau')+\ldots$$

and the response of the system is described by the expectation values on the right-hand side. However, it is seen that adding $e_\alpha(\tau)$ to the right-hand side of the equation of motion leads to the subtraction of $e_\alpha(\tau)$ from $q_\alpha(\tau)$, so that the effect of the perturbation on the expression (6) is to introduce into the integrands of numerator and denominator the factor

$$\exp\left(i\int_{t_0}^{t} d\tau\, e_\alpha(\tau)\chi_\alpha(\tau)\right).$$

Moreover, consideration of the normalization condition on the probability density P shows that the denominator is unaltered by the inclusion of this factor in the integrand. Hence we obtain

$$\delta\langle F\rangle=\frac{\int D[\psi]\int D[\chi]F[\psi](e^{i\int d\tau e_\alpha(\tau)\chi_\alpha(\tau)}-1)A[\psi,\chi]}{\int D[\psi]\int D[\chi]A[\psi,\chi]}.$$

Expanding the exponential and comparing the two series for $\delta\langle F\rangle$ shows that

$$\left\langle\frac{\delta F[\psi]}{\delta f_\alpha(\tau)}\right\rangle=\frac{\int D[\psi]\int D[\chi]i\chi_\alpha(\tau)F[\psi]A[\psi,\chi]}{\int D[\psi]\int D[\chi]A[\psi,\chi]}$$

$$\left\langle\frac{\delta^2 F[\psi]}{\delta f_\alpha(\tau)\delta f_\beta(\tau')}\right\rangle=\frac{\int D[\psi]\int D[\chi]i^2\chi_\alpha(\tau)\chi_\beta(\tau')F[\psi]A[\psi,\chi]}{\int D[\psi]\int D[\chi]A[\psi,\chi]}$$

The first-order response function of the system is defined as

$$G_{\alpha\beta}(\tau,\tau')=\left\langle\frac{\delta\psi_\alpha(\tau)}{\delta f_\beta(\tau')}\right\rangle$$

and is clearly given by

$$\frac{\int D[\psi]\int D[\chi]i\psi_\alpha(\tau)\chi_\beta(\tau')A[\psi,\chi]}{\int D[\psi]\int D[\chi]A[\psi,\chi]}.$$

The defining expression for the response function has a jump discontinuity at $\tau=\tau'$ (see below) and is not uniquely defined. If we require it to be given by the above functional integral for all τ, τ' then, in view of our definition of such integrals, the response function must be taken as half the sum of the right- and left-hand limits $\tau' \to \tau \pm 0$. Higher-order response functions are defined in the usual way:

$$G_{\alpha_1\ldots\alpha_n|\beta_1\ldots\beta_m}(\tau_1\ldots\tau_n|\tau_1'\ldots\tau_m') = \left\langle \frac{\delta^m(\psi_{\alpha_1}(\tau_1)\ldots\psi_{\alpha_n}(\tau_n))}{\delta f_{\beta_1}(\tau_1')\ldots\delta f_{\beta_m}(\tau_m')} \right\rangle$$

the functional integral representation being

$$\frac{\mathrm{i}^m \int \mathrm{D}[\psi] \int \mathrm{D}[\chi] \psi_{\alpha_1}(\tau_1)\ldots\psi_{\alpha_n}(\tau_n)\chi_{\beta_1}(\tau_1')\ldots\chi_{\beta_m}(\tau_m') A[\psi,\chi]}{\int \mathrm{D}[\psi]\int \mathrm{D}[\chi] A[\psi,\chi]}. \tag{8}$$

It is seen therefore that the functions χ which arise merely as integration variables in the work of Hosokawa and Rosen serve to generate the response functions.

We now derive an identity which will prove useful in deriving the Schwinger equations in their usual form. The equation of motion (1) may be rewritten

$$\psi_\alpha(\tau) = \int_{t_0}^{\tau} \mathrm{d}\tau'' f_\alpha(\tau'') + \int_{t_0}^{\tau} \mathrm{d}\tau'' \, \Lambda_\alpha(\psi(\tau''), \tau'').$$

Since $\psi_\alpha(\tau)$ is functionally independent of $f_\beta(\tau')$ for $\tau' > \tau$ we clearly have the causality relation

$$\delta\psi_\alpha(\tau)/\delta f_\beta(\tau') = 0$$

for $\tau < \tau'$, while for $\tau > \tau'$ we can write

$$\frac{\delta\psi_\alpha(\tau)}{\delta f_\beta(\tau')} = \delta_{\alpha\beta} + \int_{t_0}^{\tau} \mathrm{d}\tau'' \, \Lambda_{\alpha,\gamma}(\psi(\tau''), \tau'') \frac{\delta\psi_\gamma(\tau'')}{\delta f_\beta(\tau')}.$$

In view of the causality property, the integral on the right-hand side is over the range $\tau' < \tau'' < \tau$, and in the limit as $\tau' \to \tau-$ we have $\delta\psi_\alpha(\tau)/\delta f_\beta(\tau') \to \delta_{\alpha\beta}$. We shall assume that this jump discontinuity is the only discontinuity of $\delta\psi_\alpha(\tau)/\delta f_\beta(\tau')$.

We now consider the quantity

$$\frac{\delta}{\delta f_\beta(\tau')} B[\psi] h(\psi(\tau)) = \frac{\delta B[\psi]}{\delta f_\beta(\tau')} h(\psi(\tau)) + B[\psi] h_{,\gamma}(\psi(\tau)) \frac{\delta\psi_\gamma(\tau)}{\delta f_\beta(\tau')}.$$

For $\tau - \tau' \to 0+$ the right-hand side tends to

$$\frac{\delta B[\psi]}{\delta f_\beta(\tau-)} h(\psi(\tau)) + B[\psi] h_{,\beta}(\psi(\tau))$$

while for $\tau - \tau' \to 0-$ it tends to

$$\frac{\delta B[\psi]}{\delta f_\beta(\tau+)} h(\psi(\tau)).$$

If it is assumed that the functional B is such that $\delta B/\delta\psi_\beta(\tau)$ is a continuous function of τ, then so is $\delta B/\delta f_\beta(\tau)$ and the difference of the two expressions is

$$B[\psi]h_{,\beta}(\psi(\tau)).$$

If this result is expressed in terms of functional integrals we have

$$\mathrm{i}\int \mathrm{D}[\psi]\int \mathrm{D}[\chi](\chi_\beta(\tau-)-\chi_\beta(\tau+))B[\psi]h(\psi(\tau))A[\psi,\chi]$$
$$=\int \mathrm{D}[\psi]\int \mathrm{D}[\chi]B[\psi]h_{,\beta}(\psi(\tau))A[\psi,\chi]. \tag{9}$$

The same result is true if the integrand on each side of the equation is multiplied by

$$\exp\left(\mathrm{i}\int_{t_0}^{t}\mathrm{d}\tau\,\eta_\alpha(\tau)\chi_\alpha(\tau)\right)$$

since this simply corresponds to considering a different equation of motion with an extra term $\eta_\alpha(\tau)$ on the right-hand side. This identity can be used to demonstrate the equivalence of the functional integral representation given here with that derived by Hosokawa and Rosen. The appearance here of an extra factor $\exp(-\frac{1}{2}\int_{t_0}^{t}\Lambda_{\alpha,\alpha}(\psi(\tau),\tau))$ in A arises from the different definition given for the functional integral.

3. The relation with MSR theory

The next step is the introduction of a generating functional in the obvious way:

$$Z[\xi,\eta]=\frac{\int \mathrm{D}[\psi]\int \mathrm{D}[\chi]\exp[\mathrm{i}\int \mathrm{d}\tau(\xi_\alpha(\tau)\psi_\alpha(\tau)+\eta_\alpha(\tau)\chi_\alpha(\tau))]A[\psi,\chi]}{\int \mathrm{D}[\psi]\int \mathrm{D}[\chi]A[\psi,\chi]} \tag{10}$$

where the τ integration is over the interval (t_0, t) as before, and $\xi_\alpha(\tau)$, $\eta_\alpha(\tau)$ are test functions. Correlation and response functions are obtained from Z by functional differentiation:

$$U_{\alpha_1\ldots\alpha_n}(\tau_1,\ldots,\tau_n)=\frac{1}{\mathrm{i}^n}\left[\frac{\delta^n Z}{\delta\xi_{\alpha_1}(\tau_1)\ldots\delta\xi_{\alpha_n}(\tau_n)}\right]_0$$

$$G_{\alpha_1\ldots\alpha_n|\beta_1\ldots\beta_m}(\tau_1,\ldots,\tau_n|\tau_1',\ldots,\tau_m')=\frac{1}{\mathrm{i}^n}\left[\frac{\delta^{n+m}Z}{\delta\xi_{\alpha_1}(\tau_1)\ldots\delta\xi_{\alpha_n}(\tau_n)\delta\eta_{\beta_1}(\tau_1')\ldots\delta\eta_{\beta_m}(\tau_m')}\right]_0$$

where the zero outside the bracket indicates that ξ and η should be set equal to zero. In addition we have

$$[Z]_0=1.$$

From these equations it is apparent that the generating functional of MSR theory is just $Z[-\mathrm{i}\xi,\eta]$.

The Schwinger equations satisfied by Z can be obtained by simple manipulations of the functional integral (10) which can be justified for the corresponding discrete integral. Using a simplified notation for brevity we have

$$\frac{\partial}{\partial\tau}\left(\frac{1}{\mathrm{i}}\frac{\delta Z}{\delta\xi_\alpha(\tau)}\right)=\frac{\iint\dot{\psi}_\alpha(\tau)\exp[\mathrm{i}\int(\xi\psi+\eta\chi)]A}{\iint A}$$

$$=\frac{\iint(q_\alpha(\tau)+\Lambda_\alpha(\psi(\tau),\tau))\exp[\mathrm{i}\int(\xi\psi+\eta\chi)]A}{\iint A}$$

$$=\Lambda_\alpha\left(\frac{1}{\mathrm{i}}\frac{\delta}{\delta\xi(\tau)},\tau\right)Z+\frac{\iint q_\alpha(\tau)\exp[\mathrm{i}\int(\xi\psi+\eta\chi)]A}{\iint A}.$$

The numerator of the second term on the right can be written

$$\int\int \mathrm{e}^{\mathrm{i}\int(\xi\psi+\eta\chi)}C[\chi]\,\mathrm{e}^{-\frac{1}{2}\int\Lambda_{\beta,\beta}(\psi(\tau),\tau)}\mathrm{i}\frac{\delta}{\delta\chi_\alpha(\tau)}(\mathrm{e}^{-\mathrm{i}\int\chi q})$$

and performing the integration by parts gives

$$-\int\int \mathrm{e}^{-\frac{1}{2}\int\Lambda_{\beta,\beta}(\psi(\tau),\tau)}\,\mathrm{e}^{-\mathrm{i}\int\chi q}\mathrm{i}\frac{\delta}{\delta\chi_\alpha(\tau)}(C[\chi]\,\mathrm{e}^{\mathrm{i}\int(\xi\psi+\eta\chi)}).$$

If we define

$$D_\alpha([\chi],\tau)=\frac{\delta}{\delta\chi_\alpha(\tau)}\ln C[\chi]$$

this expression becomes

$$\int\int(\eta_\alpha(\tau)-\mathrm{i}D_\alpha([\chi],\tau))A[\psi,\chi]\exp\left(\mathrm{i}\int(\xi\psi+\eta\chi)\right)$$

so that the Schwinger equation becomes

$$\frac{\partial}{\partial\tau}\left(\frac{1}{\mathrm{i}}\frac{\delta Z}{\delta\xi_\alpha(\tau)}\right)=\eta_\alpha(\tau)Z+\Lambda_\alpha\left(\frac{1}{\mathrm{i}}\frac{\delta}{\delta\xi(\tau)},\tau\right)Z-\mathrm{i}D_\alpha\left(\left[\frac{1}{\mathrm{i}}\frac{\delta}{\delta\eta}\right],\tau\right)Z. \tag{11}$$

If $\ln C[\chi]$ is expanded as a functional power series

$$\frac{\mathrm{i}^2}{2!}\int\mathrm{d}\tau_1\int\mathrm{d}\tau_2\,R_{\beta\gamma}(\tau_1,\tau_2)\chi_\beta(\tau_1)\chi_\gamma(\tau_2)$$

$$+\frac{\mathrm{i}^3}{3!}\int\mathrm{d}\tau_1\ldots\int\mathrm{d}\tau_3\,M_{\beta\gamma\delta}(\tau_1,\tau_2,\tau_3)\chi_\beta(\tau_1)\chi_\gamma(\tau_2)\chi_\delta(\tau_3)+\ldots$$

where R is the second-order correlation function and M the third-order cumulant, the equation becomes

$$\frac{\partial}{\partial\tau}\left(\frac{1}{\mathrm{i}}\frac{\delta Z}{\delta\xi_\alpha(\tau)}\right)=\eta_\alpha(\tau)Z+\Lambda_\alpha\left(\frac{1}{\mathrm{i}}\frac{\delta}{\delta\xi(\tau)},\tau\right)Z+\int\mathrm{d}\tau_1\,R_{\alpha\beta}(\tau,\tau_1)\frac{\delta Z}{\delta\eta_\beta(\tau_1)}$$

$$+\frac{1}{2!}\int\mathrm{d}\tau_1\int\mathrm{d}\tau_2\,M_{\alpha\beta\gamma}(\tau,\tau_1,\tau_2)\frac{\delta^2 Z}{\delta\eta_\beta(\tau_1)\delta\eta_\gamma(\tau_2)}+\ldots.$$

For the Gaussian case the third- and higher-order cumulants vanish and the equation reduces to one previously given (Phythian 1975). It is apparent that in the diagram expansion for the non-Gaussian case 'bare' vertices of third- and higher-order will appear.

In a similar way we have

$$\frac{\partial}{\partial\tau}\left(\frac{1}{\mathrm{i}}\frac{\delta Z}{\delta\eta_\alpha(\tau)}\right)=\frac{\iint\dot{\chi}_\alpha(\tau)\exp[\mathrm{i}\int(\xi\psi+\eta\chi)]A}{\iint A}.$$

However

$$\delta A/\delta\psi_\alpha(\tau)=(-\tfrac{1}{2}\Lambda_{\beta,\beta\alpha}(\psi(\tau),\tau)+\mathrm{i}\dot{\chi}_\alpha(\tau)+\mathrm{i}\chi_\beta(\tau)\Lambda_{\beta,\alpha}(\psi(\tau),\tau))A$$

so that

$$\frac{\partial}{\partial\tau}\left(\frac{1}{\mathrm{i}}\frac{\delta Z}{\delta\eta_\alpha(\tau)}\right)$$

$$=\frac{-\mathrm{i}\iint \mathrm{e}^{\mathrm{i}\int(\xi\psi+\eta\chi)}[(\delta A/\delta\psi_\alpha(\tau))+\frac{1}{2}\Lambda_{\beta,\beta\alpha}(\psi(\tau),\tau)A-\mathrm{i}\chi_\beta(\tau)\Lambda_{\beta,\alpha}(\psi(\tau),\tau)A]}{\iint A}$$

$$=-\xi_\alpha(\tau)Z-\frac{\mathrm{i}\iint \mathrm{e}^{\mathrm{i}\int(\xi\psi+\eta\chi)}(\frac{1}{2}\Lambda_{\beta,\beta\alpha}(\psi(\tau),\tau)-\mathrm{i}\chi_\beta(\tau)\Lambda_{\beta,\alpha}(\psi(\tau),\tau))A}{\iint A}.$$

Recalling the identity (9) and the definition of integrals with simultaneous ψ and χ, the numerator of the second term on the right can be rewritten

$$-\mathrm{i}\int\int \mathrm{e}^{\mathrm{i}\int(\xi\psi+\eta\chi)}[\tfrac{1}{2}\mathrm{i}(\chi_\beta(\tau-)-\chi_\beta(\tau+))\Lambda_{\beta,\alpha}(\psi(\tau),\tau)-\tfrac{1}{2}\mathrm{i}(\chi_\beta(\tau-)+\chi_\beta(\tau+))\Lambda_{\beta,\alpha}(\psi(\tau),\tau)]A$$

$$=-\int\int \mathrm{e}^{\mathrm{i}\int(\xi\psi+\eta\chi)}\chi_\beta(\tau+)\Lambda_{\beta,\alpha}(\psi(\tau),\tau)A.$$

The second Schwinger equation then becomes

$$\frac{\partial}{\partial\tau}\left(\frac{1}{\mathrm{i}}\frac{\delta Z}{\delta\eta_\alpha(\tau)}\right)=-\xi_\alpha(\tau)Z+\mathrm{i}\frac{\delta}{\delta\eta_\beta(\tau+)}\Lambda_{\beta,\alpha}\left(\frac{1}{\mathrm{i}}\frac{\delta}{\delta\xi(\tau)},\tau\right)Z. \tag{12}$$

4. More general equation of motion

We now consider a more complicated equation of motion

$$\dot{\psi}_\alpha(\tau)=f_\alpha(\tau)+g_\beta(\tau)\Gamma_{\beta\alpha}(\psi(\tau),\tau)+\Lambda_\alpha(\psi(\tau),\tau)$$

where f and g are random functions of zero mean whose probability distribution is specified by the joint characteristic functional

$$C[\phi,\rho]=\left\langle\exp\left(\mathrm{i}\int_{t_0}^{t}\mathrm{d}\tau(\phi_\alpha(\tau)f_\alpha(\tau)+\rho_\alpha(\tau)g_\alpha(\tau))\right)\right\rangle.$$

The simplest way to derive the functional integral representation in this case is to imagine the functions g held fixed so that the above method may be used, and then to perform the further averaging over g. The formula (6) remains true with A now given by

$$A[\psi,\chi]=\exp\left(-\tfrac{1}{2}\int_{t_0}^{t}\mathrm{d}\tau\,\Lambda_{\alpha,\alpha}(\psi(\tau),\tau)-\mathrm{i}\int_{t_0}^{t}\mathrm{d}\tau\,\chi_\alpha(\tau)(\dot{\psi}_\alpha(\tau)-\Lambda_\alpha(\psi(\tau),\tau))\right)$$

$$\times C[\chi,\Gamma\chi+\mathrm{i}\,\mathrm{div}\,\Gamma]$$

where

$$\rho = \Gamma\chi + \mathrm{i}\,\mathrm{div}\,\Gamma$$

is an abbreviated notation for

$$\rho_\alpha(\tau) = \Gamma_{\alpha\beta}(\psi(\tau), \tau)\chi_\beta(\tau) + \mathrm{i}\Gamma_{\alpha\beta,\beta}(\psi(\tau), \tau).$$

As before the functional integral is defined as the limit of a discrete integral of a function of the variables $\psi(t_1), \ldots, \psi(t_N)$; $\chi(t_1^*), \ldots, \chi(t_N^*)$, and the rule for treating simultaneous ψ and χ remains the same.

The response to non-random perturbations of f is given as before by (8) using the new form of A. It is of interest to consider also the response to perturbations of g. The effect of adding $e_\alpha(\tau)$ to $g_\alpha(\tau)$ is to replace $q_\alpha(\tau)$ in the expression for A by

$$q_\alpha(\tau) - e_\beta(\tau)\Gamma_{\beta\alpha}(\psi(\tau), \tau)$$

and proceeding as before we obtain finally

$$\left\langle \frac{\delta F[\psi]}{\delta g_\alpha(\tau)} \right\rangle = \frac{\mathrm{i}\int \mathrm{D}[\psi] \int \mathrm{D}[\chi]\chi_\beta(\tau+)\Gamma_{\alpha\beta}(\psi(\tau), \tau)F[\psi]A[\psi, \chi]}{\int \mathrm{D}[\psi] \int \mathrm{D}[\chi] A[\psi, \chi]}$$

$$\left\langle \frac{\delta^2 F[\psi]}{\delta g_\alpha(\tau)\delta g_\beta(\tau')} \right\rangle$$

$$= \frac{\mathrm{i}^2 \int \mathrm{D}[\psi] \int \mathrm{D}[\chi]\chi_\gamma(\tau+)\Gamma_{\alpha\gamma}(\psi(\tau), \tau)\chi_\delta(\tau'+)\Gamma_{\beta\delta}(\psi(\tau'), \tau')F[\psi]A[\psi, \chi]}{\int \mathrm{D}[\psi] \int \mathrm{D}[\chi] A[\psi, \chi]}.$$

The generating functional is defined as before and the Schwinger equation obtained by manipulations of the defining integral. We obtain

$$\frac{\partial}{\partial\tau}\left(\frac{1}{\mathrm{i}}\frac{\delta Z}{\delta\xi_\alpha(\tau)}\right) = \eta_\alpha(\tau) + \Lambda_\alpha\left(\frac{1}{\mathrm{i}}\frac{\delta}{\delta\xi(\tau)}, \tau\right)Z - \mathrm{i}D_\alpha\left(\left[\frac{1}{\mathrm{i}}\frac{\delta}{\delta\xi}\right], \left[\frac{1}{\mathrm{i}}\frac{\delta}{\delta\eta}\right], \tau\right)Z$$

$$\frac{\partial}{\partial\tau}\left(\frac{1}{\mathrm{i}}\frac{\delta Z}{\delta\eta_\alpha(\tau)}\right) = -\xi_\alpha(\tau)Z - \frac{\mathrm{i}}{2}\Lambda_{\beta,\beta\alpha}\left(\frac{1}{\mathrm{i}}\frac{\delta}{\delta\xi(\tau)}, \tau\right)Z + \mathrm{i}\frac{\delta}{\delta\eta_\beta(\tau)}\Lambda_{\beta,\alpha}\left(\frac{1}{\mathrm{i}}\frac{\delta}{\delta\xi(\tau)}, \tau\right)Z$$

$$+\mathrm{i}E_\alpha\left(\left[\frac{1}{\mathrm{i}}\frac{\delta}{\delta\xi}\right], \left[\frac{1}{\mathrm{i}}\frac{\delta}{\delta\eta}\right], \tau\right)Z$$

where

$$D_\alpha([\psi], [\chi], \tau) = \frac{\delta}{\delta\chi_\alpha(\tau)} \ln C[\chi, \Gamma\chi + \mathrm{i}\,\mathrm{div}\,\Gamma]$$

$$E_\alpha([\psi], [\chi], \tau) = \frac{\delta}{\delta\psi_\alpha(\tau)} \ln C[\chi, \Gamma\chi + \mathrm{i}\,\mathrm{div}\,\Gamma].$$

The rule for treating integrals with simultaneous ψ and χ implies a similar rule for the simultaneous derivatives $\delta/\delta\xi(\tau)$, $\delta/\delta\eta(\tau)$. For the particular case in which f and g are independent Gaussian random functions these equations can be expressed in a form derived previously (Phythian 1976).

5. Discussion

It has been demonstrated that the functional integral representation provides the simplest approach to the derivation of Schwinger equations and hence of the associated diagram formalism. In addition it can suggest approximations which are difficult to formulate by any other means. Two possibilities which come to mind are the extremal path approximation and the Feynman variational method. However, the functional integral given here is not in a form suitable for the application of these methods. To see this more clearly let us consider the quantity A given by (7) for the Gaussian case with correlation function R. We have

$$A[\psi,\chi]=\exp\Big(-\tfrac{1}{2}\int \mathrm{d}\tau\ \Lambda_{\alpha,\alpha}(\psi(\tau),\tau)-\mathrm{i}\int \mathrm{d}\tau\,\chi_\alpha(\tau)(\dot\psi_\alpha(\tau)-\Lambda_\alpha(\psi(\tau),\tau)) -\tfrac{1}{2}\int \mathrm{d}\tau\int \mathrm{d}\tau'\,R_{\alpha\beta}(\tau,\tau')\chi_\alpha(\tau)\chi_\beta(\tau')\Big)$$

and it is seen that the exponent is neither real nor pure imaginary. A real exponent is necessary for the application of the Feynman variational method, as for example in equilibrium statistical mechanics (Feynman and Hibbs 1965). Similarly the interpretation of the extremal path approximation is not clear since, whereas the integration extends only over real functions, the extremal will not in general be attained for real functions. A similar question arising in a different context has been discussed by McLaughlin (1972).

These difficulties can be avoided in the Gaussian case by performing the χ integration explicitly. Ignoring the normalization constant the integral for $\langle F\rangle$ then assumes the form

$$\int \mathrm{D}[\psi]F[\psi]\exp\Big(-\tfrac{1}{2}\int_{t_0}^{t}\Lambda_{\alpha,\alpha}(\psi(\tau),\tau)-\tfrac{1}{2}\int_{t_0}^{t}\mathrm{d}\tau\int_{t_0}^{t}\mathrm{d}\tau'\,Q_{\alpha\beta}(\tau,\tau')q_\alpha(\tau)q_\beta(\tau')\Big)$$

where Q is the inverse of R (assumed non-singular)

$$\int_{t_0}^{t}\mathrm{d}\tau'\,Q_{\alpha\beta}(\tau,\tau')R_{\beta\gamma}(\tau',\tau'')=\delta_{\alpha\gamma}\delta(\tau-\tau'').$$

If $F\equiv 1$ and the integral is evaluated over all trajectories with $\psi(t_0)$ and $\psi(t)$ taking prescribed values it gives the joint probability density for the dynamical variables at time t. This form of the integral is analogous to the Feynman path integral

$$\int \mathrm{D}[x]\exp\Big[\mathrm{i}\int_{t_0}^{t}\mathrm{d}\tau\Big(\frac{(\dot x(\tau))^2}{2m}-V(x(\tau))\Big)\Big]$$

while the original form is the analogue of

$$\int \mathrm{D}[x]\int \mathrm{D}[p]\exp\Big[\mathrm{i}\int_{t_0}^{t}\mathrm{d}\tau\Big(p(\tau)\dot x(\tau)-\frac{1}{2m}p^2(\tau)-V(x(\tau))\Big)\Big]$$

(see Katz 1965). The condition for an extremal value of the exponent with fixed end points can be written in the form

$$\dot\psi_\alpha(\tau)=\Lambda_\alpha(\psi(\tau),\tau)+\int_{t_0}^{t}\mathrm{d}\tau'\,R_{\alpha\beta}(\tau,\tau')\hat\psi_\beta(\tau')$$

$$\dot{\hat\psi}_\alpha(\tau)=-\hat\psi_\beta(\tau)\Lambda_{\beta,\alpha}(\psi(\tau),\tau)+\Lambda_{\beta,\beta\alpha}(\psi(\tau),\tau)$$

where we have defined $\hat{\psi}$ by the equation

$$\hat{\psi}_\alpha(\tau)=\int_{t_0}^{t} d\tau'\, Q_{\alpha\beta}(\tau,\tau')(\dot{\psi}_\beta(\tau')-\Lambda_\beta(\psi(\tau'),\tau')).$$

Not surprisingly these equations are similar to those which appear in the operator theory. If it is assumed that the extremal value corresponds to a strong maximum of the exponential, a good approximation will be given by retaining in the exponent terms up to second order in the departure of a trajectory from the most probable one. The details are similar to those involved in the discussion of the quasi-classical approximation of quantum mechanics. There still remains the integration over the amplitudes at time t if correlations are to be calculated so the method is likely to be useful only if the number of modes is small unless further approximations are made. This method has recently been applied to the problem of wave propagation in random media by Chow (1972).

The Feynman variational method (Feynman and Hibbs 1965) is based on the inequality

$$\int D[\psi]\, e^{S[\psi]} \geqslant e^{\langle S-B\rangle}\int D[\psi]\, e^{B[\psi]}$$

where $\langle S-B\rangle$ denotes

$$\frac{\int D[\psi](S[\psi]-B[\psi])\, e^{B[\psi]}}{\int D[\psi]\, e^{B[\psi]}}.$$

If B is chosen as a quadratic functional, the integrals on the right can be performed provided that S is a polynomial functional. By varying B to maximize the right-hand side a lower bound is obtained which in some cases can give a useful approximation.

Another approximation closely related to the one just described is given by Siegel and Burke (1972). This gives what is essentially a perturbation theory treatment of the non-linear terms of the equation of motion, but differs from the usual perturbation theory in that the average of these terms, defined in terms of a suitable function space integral, is first subtracted out. This method can be applied to either form of the functional integral representation.

The functional integral representation would therefore seem to merit further investigation and we hope to give a fuller discussion of these ideas in a later work.

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