Ref.TH.3864-CERN

STOCHASTIC QUANTIZATION AS A CONSEQUENCE OF
THE MICROCANONICAL ENSEMBLE

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A B S T R A C T

It is shown that the concept of stochastic quantization arises naturally within the framework of a microcanonical ensemble formulation of quantum field theory. Various parallels in the two schemes are also explored.

Ref.TH.3864-CERN

April 1984

1. PROLOGEMENA

One of the most interesting recent ideas in quantum field theory is the concept of stochastic quantization¹⁾. In this formulation of field theory, expectation values of various operators are calculated by solving a first-order differential equation which includes a random noise term. Within the new framework it is possible to avoid the Gribov ambiguity²⁾ while otherwise obtaining results equivalent³⁾ to those calculated by standard methods.

Another formulation^{4),5)} of quantum field theory, derived from the microcanonical ensemble of classical statistical mechanics, has also been presented recently. In the microcanonical ensemble, expectation values are calculated by solving a second-order ordinary (as opposed to partial) differential equation. Various technical advantages of this new ensemble over standard Monte Carlo methods (especially for computations involving fermions) were suggested in the initial work⁴⁾; subsequent calculations^{5),6)} using the new formalism seem to bear out this optimism. An alternative microcanonical formulation of field theory⁷⁾ also shows some promise.

Interestingly enough, there is a direct connection between the stochastic and microcanonical methods; the former involving a first-order differential equation in the presence of a stochastic noise term, and the latter using a second-order differential equation with no noise term. The aforementioned connection, which requires a brief journey through the standard lore of statistical mechanics, is explored in the sequel.

2. FROM THE MICROCANONICAL ENSEMBLE

It is convenient to review first the microcanonical ensemble formulation of quantum field theory and then demonstrate how the idea of stochastic quantization arises naturally within this framework. For simplicity in dealing with the path integrals displayed below, it is tacitly assumed that the theory is formulated upon a lattice in Euclidean space-time. Presumably taking the continuum limit of such a theory presents no problems of principle.

The system of fields $\{\phi\}$ is governed by an action

$$S\{\phi\} = \beta V\{\phi\} , \quad (1)$$

where β is an overall coupling constant of the theory (for example, in a lattice gauge theory $\beta \sim (g_0)^{-2}$, with g_0 the bare coupling constant). Expectation values of operators $O\{\phi\}$ in the standard path integral formalism are given by the formula

$$\langle O \rangle \equiv \frac{\int D\phi \ O\{\phi\} \exp[-\beta V\{\phi\}]}{\int D\phi \ \exp[-\beta V\{\phi\}]} , \quad (2)$$

where $D\phi$ refers to the standard functional measure.

Any quantity independent of all the $\{\phi\}$ can be added to the action $S\{\phi\}$ without affecting the expectation value of any functional of the $\{\phi\}$. Hence, it follows that

$$\begin{aligned} \langle O \rangle &= \langle O \rangle_{\text{canon}} = Z_{\text{canon}}^{-1} \int Dp \int D\phi \ e^{-\beta H} O\{\phi\} , \\ Z_{\text{canon}} &\equiv \int Dp \int D\phi \ e^{-\beta H} , \end{aligned} \quad (3)$$

$$H = T + V , \quad T = \sum_{\vec{i}} p_{\vec{i}}^2 ,$$

where the notation has been chosen in such a fashion as to suggest a connection with the canonical ensemble of statistical mechanics.

This connection can be turned into an isomorphism with the identification

$$\frac{d\phi_{\vec{i}}}{d\tau} = p_{\vec{i}} , \quad (4)$$

provided that a new "artificial time" co-ordinate τ is introduced⁸⁾. A Lagrangian formulation of an Euclidean quantum field theory embedded in d dimensions is thus mapped to a "Hamiltonian" formalism in $d+1$ dimensions.

Equations (3) define a canonical ensemble with kinetic energy T , potential energy V , and temperature β^{-1} . This ensemble describes the states of a system (governed by a Hamiltonian $H\{p, \phi\}$) in contact with a heat bath at fixed temperature β^{-1} .

A microcanonical ensemble⁹⁾ on the other hand describes a system in thermal isolation, and hence the "energy" $H\{p, \phi\}$ of the system is constrained to equal a fixed value E , while the temperature β^{-1} is defined as the average kinetic energy (suitably normalized). Each co-ordinate evolves in the artificial time τ according to Hamilton's equation

$$\frac{d^2 \phi_i}{d\tau^2} = \frac{d p_i}{d\tau} = - \frac{\partial V\{\phi\}}{\partial \phi_i} \quad . \quad (5)$$

Formally, expectation values in the microcanonical ensemble are written as

$$\langle \theta \rangle_{\text{micro}} \equiv Z_{\text{micro}}^{-1} \int Dp \int D\phi \, \theta\{p, \phi\} \delta(H-E) \quad (6.a)$$

with

$$Z_{\text{micro}} \equiv \int Dp \int D\phi \, \delta(H-E) \quad . \quad (6.b)$$

The integrals in Eqs. (6) are over the hypersurface of constant "energy", $H\{p, \phi\} = E$.

The expectation value of any functional of the $\{p\}$ and the $\{\phi\}$ can be calculated by using the $\{p(\tau)\}$ and $\{\phi(\tau)\}$ generated along the trajectory given by the solution of Eqs. (5). Any expectation value is thus given by

$$\langle O \rangle_{\text{micro}} = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau d\tau' O\{p(\tau'), \psi(\tau')\} , \quad (7)$$

and is a unique function of E.

The equivalence of Eqs. (6) and (7) follows from a vital assumption of ensemble theory known as the principle of equal weight¹⁰⁾. This principle assures us that for a given E, the trajectories given by the solution of Eqs. (5) cover surfaces of constant E in the phase space $\{p, \phi\}$ with equal density. The additional assumption that all expectation values of a physical system can be computed in either ensemble is discussed and partially proven in Ref. 11).

The average "kinetic energy" $\langle T \rangle$ which defines the analogue temperature β^{-1} is given by

$$\beta^{-1} = \frac{2}{N} \langle T \rangle_{\text{micro}} = \langle \dot{\varphi}_i^2 \rangle_{\text{micro}} , \quad (8)$$

where N is the number of independent degrees of freedom in the system. [For gauge theories special care in counting these degrees of freedom is required. See Refs. 4) and 5).]

3.TO STOCHASTIC QUANTIZATION

The derivation of stochastic quantization from the microcanonical ensemble is an elementary exercise once the proper physical concepts are at hand. The difference between the two is essentially one of time scale, and can be illustrated by a simple picture.

Imagine a large set of classical particles colliding elastically. Denote the mean time between collisions (i.e., the correlation time) by ϵ . If many observations separated by intervals of time much less than ϵ are made, then the picture which emerges is one of smooth, deterministic, conservative movement -- in other words, the microcanonical ensemble.

On the other hand, if observations are made at time intervals much larger than ϵ (or if the motion is averaged over this larger time scale) a quite different picture emerges -- that of chaotic, random motion. This difference comes about because in large ergodic systems information about the past trajectory of a particle is lost after a few collisions. (This description oversimplifies the situation. What actually happens is that the present position and momentum of each particle must be known with perfect precision in order to recover the entire past history of the ensemble.) Of course, this latter case corresponds to stochastic quantization.

These ideas can be formulated quantitatively. Consider the (artificial) time correlation function of two momenta in the microcanonical ensemble:

$$\langle P_i(\tau) P_j(0) \rangle_{\text{ens}} = \beta^{-1} \delta_{ij} C(\tau) \quad , \quad (9)$$

where the brackets $\langle \rangle_{\text{ens}}$ refer to an "ensemble" average over an infinite number of thermodynamically equivalent systems. It is assumed here that this average equals the microcanonical average Eq. (7), (i.e., that the system is ergodic).

Given that a "correlation time" ϵ can be defined by

$$\int_{-\infty}^{\infty} d\tau C(\tau) = 2\epsilon \quad , \quad (10)$$

it is assumed below that $C(\tau)$ is zero if $|\tau|$ is much greater than ϵ . Thus if $C(\tau)$ is measured over time scales much larger than ϵ , it will be observed that

$$C(\tau) d\tau \rightarrow 2\epsilon \delta(\tau) d\tau \quad . \quad (11)$$

A pedagogically convenient (though overly simplified) model for $C(\tau)$ is:

$$C(\tau) = \exp(-|\tau|/\epsilon) \quad . \quad (12)$$

This model is suggested for illustration only, and is not needed for the following discussion.

Next consider Eq. (5), which defines the trajectories $\{p(\tau), \phi(\tau)\}$ in the microcanonical ensemble. If this equation is integrated from $\tau-\varepsilon$ to τ the result can be written

$$p_i(\tau) = \frac{d\phi_i(\tau)}{d\tau} = - \left[\int_{\tau-\varepsilon}^{\tau} \frac{\partial V}{\partial \phi_i} d\tau \right] + p_i(\tau-\varepsilon) \quad (13)$$

During the interval ε , the fields $\{p\}$ become essentially independent of their initial values, and so $p_i(\tau)$ is uncorrelated with $p_i(\tau-\varepsilon)$. This process occurs in a smooth and analytic fashion, so if the ensemble is observed over time scales large compared with ε , it is reasonable to expand the integral in Eq. (13) for small ε . The result can be written (with ε^2 corrections dropped):

$$\frac{d\phi_i}{ds} = - \frac{\partial V}{\partial \phi_i} + \eta_i(s) \quad \bullet \quad (14)$$

In Eq. (14) several redefinitions have been made:

$$\begin{aligned} s &\equiv \varepsilon \tau \\ \eta(s) &\equiv \varepsilon^{-1} p(\tau-\varepsilon) \end{aligned} \quad \bullet \quad (15)$$

From Eqs. (9) and (11), it follows that for time scales much larger than ε ,

$$\langle \eta_i(s) \eta_j(0) \rangle = 2\beta^{-1} \delta_{ij} \delta(s) \quad \bullet \quad (16)$$

Equations (14) to (16) are easily recognized as the defining equations for stochastic quantization¹⁾.

An interesting point which follows from Eqs. (15) is the fact that the artificial time co-ordinate s used in stochastic quantization differs by a factor of ϵ from the artificial time τ used in the microcanonical ensemble. This difference may lead one to speculate that one method can be shown to be computationally faster than the other (depending on the value of ϵ for the system under consideration) since time "runs faster" in one system. The argument of time scale is not obviously relevant, however, since it is the rate at which configuration space is covered (and not the intrinsic unit of time) that determines the computational efficiency of an algorithm. In fact, explicit calculations^{4),5)} suggest that the difference in computational speed is not dramatic in typical cases.

A word of caution is in order. In making the connection between the microcanonical ensemble and stochastic quantization, the equivalence of the microcanonical (or time) average and the ensemble average is assumed. Of course, this equivalence requires ergodic behaviour for the solutions of the differential equations, (5). If on the other hand the potential $V\{\phi\}$ is quadratic in the fields $\{\phi\}$, the resulting equations of motion describe a coupled set of harmonic oscillators and are not ergodic. Thus for example the extraction of a perturbation expansion about a free field theory (although formally seemingly consistent) would break down because the free-field limit is not ergodic, and hence Eq. (9) cannot hold. Essentially, what is needed for ergodic behaviour is that the momenta $\{p\}$ act as white-noise sources (i.e., have an almost frequency-independent spectrum) at least up to frequencies of order $1/\epsilon$.

In conclusion, it has been shown that stochastic quantization is a natural consequence of the microcanonical ensemble formulation of quantum field theory given certain standard assumptions of ergodicity. Various features of the two methods were shown to emerge as a consequence of the analysis.

It is a pleasure to thank J. Polonyi for a useful conversation.

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