Stochastic Quantization of Constrained Systems
—— General Theory and Nonlinear Sigma Model ——

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The stochastic quantization method is extended to a dynamical system described by regular Lagrangian under additional holonomic constraints. We first show that the stochastic quantization method surely yields the same result as given by the path-integral quantization, by imposing the constraints on the system throughout the whole hypothetical stochastic process with respect to a fictitious time. Next we propose, on the analogy of the theory of optimization, new types of rather moderate constraints, (i) converging constraints and (ii) fluctuating constraints, which are so designed as to coincide with the original ones only at the infinite fictitious-time limit. The present formalism with the new types of constraints prepares a feasible method to carry out numerical analyses of a dynamical system with nonlinear constraints. We can expect that the method works well in the case of the lattice nonlinear $\sigma$-model.

§1. Introduction

In previous papers we have seen remarkable merits of the stochastic quantization method originally proposed by Parisi and Wu.\(^1\) Especially, it is stressed that the stochastic quantization method enables us to quantize the non-Abelian gauge field without resort to introduction of the conventional gauge-fixing term into Lagrangian and to produce the so-called Faddeev-Popov ghost effects without resort to artificial input of any ghost field.\(^2\) Furthermore we have formulated a sort of covariant gauge-fixing condition which gives automatically the Faddeev-Popov ghost effects without help of any ghost field, as a non-holonomic constraint to be imposed on the basic Langevin equation within the framework of the stochastic quantization method.\(^3\) It appears that the stochastic quantization method can really enlarge the territory of quantum mechanics beyond the one given by the conventional quantization methods. In order to develop it further, especially, its non-perturbative approach to the field theory, it would be important to examine applicability or utility of the stochastic quantization method for dynamical systems with nonlinear constraints, because it is not so easy to quantize such systems by means of the conventional quantization methods. In this paper we attempt to formulate, as the first step, the stochastic quantization of a dynamical system described by regular Lagrangian under additional holonomic constraints.

As is well known, the stochastic quantization method prepares a simple prescription to derive the Euclidean field-theoretical propagator from the corresponding correlation function of a random field $\phi(x, t)$, depending on a fictitious time $t$ besides 4-dimensional Euclidean space-time coordinate $x$, by the formula

$$\Delta(x-x')=\lim_{t' \to t} \langle \phi(x', t') \phi(x', t') \rangle_{t=t'}$$

for instance. Here $\phi(x, t)$ obeys a Langevin equation of the form

$$\frac{\partial}{\partial t} \phi(x, t) = -\frac{\delta S[\phi]}{\delta \phi} \bigg|_{\phi=\phi(x,t)} + \eta(x, t)$$

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to describe a hypothetical stochastic process with respect to \( t \), where \( S[\phi] \) stands for the action functional and \( \eta \) for a Gaussian white-noise source. If the Lagrangian to give \( S \) is regular, Eq. (1·2) gives a definite equilibrium distribution functional proportional to \( \exp\{-S[\phi]\} \) which is the same measure with respect to \( \phi \) as in the path-integral quantization. Thus the prescription of the stochastic quantization method is well posed for regular Lagrangians. We are, however, interested here in stochastic quantization of those constrained systems which cannot be described by any regular Lagrangian. Especially, in this paper we discuss stochastic quantization of a dynamical system having originally a regular Lagrangian under additional holonomic constraints, whose Lagrangian modified by Lagrange multipliers becomes singular. To do this, first of all, we should discuss how to impose the constraints on the basic Langevin equation.

A naive way of introducing holonomic constraints into the stochastic quantization method is to impose them on the basic Langevin equation, time by time, throughout the whole hypothetical stochastic process with respect to fictitious time \( t \). We call it time-by-time constraints in what follows. In §2 it is explicitly shown that the stochastic quantization method can reproduce the conventional path-integral measure for constrained systems under the time-by-time constraints. Nevertheless, this type of constraint is not so convenient for numerical analyses, as will be seen in §3 in the case of the lattice nonlinear sigma model. In order to improve the situation, in §4, we propose to use new types of constraints, named (i) converging constraints and (ii) fluctuating constraints, which are so designed as to coincide with the original constraints only at the infinite fictitious-time limit. They are suggested by the recent developments in the theory of optimization. The new types of constraint are characterized by additional constraint forces to prevent the system from walking out of the constraint surfaces.

§ 2. Equilibrium distribution of constrained systems

For the sake of convenience, consider a dynamical system with \( N \) degrees of freedom which is described by coordinates \( q=(q_1, \cdots, q_N) \) and regular Lagrangian \( L(q, dq/dx_0) \), \( x_0 \) being the real time, under a set of holonomic constraints

\[ F^a(q)=0. \quad (a=1, \cdots, M) \quad (2·1) \]

Note that \( N>M \). It is easy to generalize the formalism to field theory with infinite degrees of freedom. According to the standard prescription of the canonical formalism, we can deal with such a system by means of a singular Lagrangian

\[ L(q, dq/dx_0, \lambda)=L(q, dq/dx_0)+\sum_{a=1}^M \lambda^a F^a(q), \quad (2·2) \]

\( \lambda=(\lambda_1, \cdots, \lambda_M) \) being Lagrange multipliers. Lagrangian (2·2) implies that we have constraints of the second class, \( \chi^{(a)}(\phi, \pi, q, \lambda)=0 \) (\( \mu=1, \cdots, 4M \) in this case), where \( \phi \) and

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*) Equivalence of the stochastic quantization to the conventional one and other properties have been discussed in detail in the papers in Ref. 4).

**) After the completion of the manuscript we found a paper of Aldazabal and Parga,¹ which deals with the nonlinear \( \sigma \)-model by means of the stochastic quantization method under the time-by-time constraints in a way quite different from ours. However, they have never discussed those new types of constraint which we propose in this paper.
\(\pi_a\) are canonical momenta conjugate to \(q_i\) and \(\lambda_a\), respectively. See Appendix A. It is well known that the system can be quantized to give a quantum mechanical transition amplitude in the path-integral representation as follows:\(^{3}\)

\[
\langle f|i \rangle = \int \Pi_i d\pi_i d\lambda_a d\pi_a \exp \left[ i \int dx_0 \left( \pi_i \frac{dq_i}{dx_0} + \pi_a \frac{d\lambda_a}{dx_0} - H_T \right) \right] \times \prod p \delta(x_\mu) \sqrt{\det \{x_\mu, x_\nu\}},
\]

(2.3)
apart from the normalization constant, where \(\{ \cdots \} \) represents a Poisson-bracket with respect to the canonical variables \(p, \pi, q\), and \(\lambda\), and \(H_T\) is defined in Appendix A. From now on we suppress summation symbols \(\Sigma_{i=1}^N\) and \(\Sigma_{a=1}^M\) over dummy indices \(i\) and \(a\).

Integrating over \(p, \pi\) and \(\lambda\), and going to Euclidean space, we get the following Lagrangian path-integral formula:

\[
\langle f|i \rangle = \int \Pi_i dq_i \exp \left[ \int dx E \right] \prod_a \delta(F^a(q)) \sqrt{\det \left( \frac{\partial F^a}{\partial q_i} \frac{\partial F^b}{\partial q_i} \right)}
\]

(2.4)
apart from the normalization constant, as shown in Appendix A, where \(x_i\) and \(L_E\), respectively, are Euclidean time and Euclidean Lagrangian. We have assumed that the matrix defined by

\[
D^{ab} = \frac{\partial F^a}{\partial q_i} \frac{\partial F^b}{\partial q_i}
\]

(2.5)
is positive and not singular.

Our problem is to derive Eq. (2.4) within the framework of the stochastic quantization method. As was mentioned in §1, a naive way of introducing the constraints into the stochastic quantization method is to impose directly Eq. (2.1) itself on the basic Langevin equation in the following way:

\[
\begin{align*}
\dot{q}_i &= -\left( \frac{\delta S}{\delta q_i} + \lambda^a \frac{\partial F^a}{\partial q_i} \right) + \eta_i, \quad (i = 1, \ldots, N) \quad (2.6a) \\
F^a(q_i(t)) &= 0, \quad (a = 1, \ldots, N) \quad (2.6b)
\end{align*}
\]

\(\eta\) being the Gaussian white noise characterized by

\[
\langle \eta_i(t) \rangle = 0, \quad \langle \eta_i(t) \eta_j(t') \rangle = 2\delta_{ij} \delta(t-t')
\]

(2.6c)
and \(\delta S/\delta q_i\), the Euler derivative of action \(S = \int dx L_E\). This type of constraints, Eq. (2.6b), imposed on the Langevin equation may be called time-by-time constraints. Since the time-by-time constraints are imposed over the whole hypothetical stochastic process with respect to fictitious time \(t\), we should have the consistency condition

\[
\frac{\partial F^a}{\partial q_i} \dot{q}_i = 0.
\]

(2.7)

From Eqs. (2.6a) and (2.7) we can easily get

\[
\lambda^a = (D^{-1})^{ab} \frac{\partial F^b}{\partial q_i} \left( -\frac{\delta S}{\delta q_i} + \eta_i \right)
\]

(2.8)
where \(D^{-1}\) is the inverse of matrix \(D\) given by Eq. (2.5). Substituting Eq. (2.8) into
Eq. (2.6a), we obtain
\[ \dot{q}_i = \frac{\partial F^a}{\partial q_i} (D^{-1})^{ab} \frac{\partial F^b}{\partial q_j} \left( - \frac{\delta S}{\delta q_j} + \eta_j \right). \]  
(2.9)

By making use of projection matrices \( P \) and \( R \) defined with
\[ P_{ij} = \delta_{ij} - \frac{\partial F^a}{\partial q_i} (D^{-1})^{ab} \frac{\partial F^b}{\partial q_j}, \]  
\[ R_{ij} = \frac{\partial F^a}{\partial q_i} (D^{-1})^{ab} \frac{\partial F^b}{\partial q_j}, \]  
(2.10)

Eq. (2.9) can be decomposed into two equations:
\[ P_{ij} \dot{q}_j = P_{ij} \left( - \frac{\delta S}{\delta q_j} + \eta_j \right), \]  
(2.11a)
\[ R_{ij} \dot{q}_j = 0, \]  
(2.11b)

where we have used \( P + R = I, \ P^2 = P, \ R^2 = R \) and \( PR = 0 \). Since \( P \) and \( R \) are, respectively, projection matrices of rank \( N - M \) and \( M \) because \( \text{Tr}(P) = N - M \) and \( \text{Tr}(R) = M \), we know that the whole manifold \( \mathcal{M}^N \) spanned by \( q = (q_1, \ldots, q_N) \) can be decomposed into the \((N-M)\)-dimensional submanifold \( \mathcal{M}^{N-M} = P \mathcal{M}^N \) and the \( M \)-dimensional submanifold \( \mathcal{M}^M = R \mathcal{M}^N : \mathcal{M}^N = \mathcal{M}^{N-M} + \mathcal{M}^M \) and \( \mathcal{M}^{N-M} \perp \mathcal{M}^M \). We may call \( \mathcal{M}^{N-M} \) constraint surface. Note that Eqs. (2.11a) and (2.11b) read the Langevin equations in \( \mathcal{M}^{N-M} \) and in \( \mathcal{M}^M \), respectively, although the latter becomes deterministic.

In order to diagonalize \( P \) and \( R \), we first introduce a set of vectors \( \{ u^{(a)} \} \) and its reciprocal set \( \{ v^{(a)} \} \) defined by
\[ u_i^{(a)} = \frac{\partial F^a}{\partial q_i}, \quad v_i^{(a)} = (D^{-1})^{ab} \frac{\partial F^b}{\partial q_i} \quad (a = N - M + 1, \ldots, N) \]  
(2.12)*

in manifold \( \mathcal{M}^M \), which satisfy the orthonormal and completeness conditions
\[ u_i^{(a)} v_i^{(b)} = \delta_{ab}, \quad u_i^{(a)} v_j^{(a)} = \delta_{ij} - P_{ij}. \]  
(2.13)

Here it should be remarked that we are quite free to select an arbitrary set of fundamental vectors \( \{ u^{(A)} \} \) \((A = 1, \ldots, N - M)\) in \( \mathcal{M}^{N-M} \) under the condition
\[ u_i^{(A)} v_i^{(a)} = 0 \quad (A = 1, \ldots, N - M; \ a = N - M + 1, \ldots, N) \]  
(2.14)
in \( \mathcal{M}^N \). Fix one set of fundamental vectors, i.e., \( \{ u^{(A)} \} \), then we can determine its metric by
\[ d^{AB} = u_i^{(A)} u_i^{(B)}, \]  
(2.15)

which gives a reciprocal set \( \{ v^{(A)} \} \) defined by
\[ v_i^{(A)} = (d^{-1})^{AB} u_i^{(B)}. \]  
(2.16)

We also assume that matrix \( (d^{AB}) \) is positive and not singular. It is easy to see that
\[ u_i^{(A)} v_i^{(B)} = \delta_{AB}, \quad u_i^{(A)} v_j^{(A)} = \delta_{ij} - R_{ij}. \]  
(2.17)

*1 Note that we have recounted \( a \) and \( b \) from \( N - M + 1 \) to \( N \), for later convenience, rather than the original range from 1 to \( M \).
Furthermore note that we have

$$u_t^{(A)} u_t^{(a)} = v_t^{(A)} v_t^{(a)} = 0 \quad (A=1, \ldots, N-M, a=N-M+1, \ldots, N)$$

(2.18)

because of $A_{N-M} \perp A^M$ or of Eqs. (2.12), (2.14) and (2.16).

Now we are able to assemble $\{u^{(A)}\}$ and $\{u^{(a)}\}$ into a set of fundamental vectors

$$\{e^\mu\} = \{u^{(1)} \ldots, u^{(N-M)}, u^{(N-M+1)}, \ldots, u^{(N)}\}$$

(2.19a)

and $\{v^{(A)}\}$ and $\{v^{(a)}\}$ into its reciprocal set

$$\{e_\mu\} = \{v^{(1)} \ldots, v^{(N-M)}, v^{(N-M+1)}, \ldots, v^{(N)}\}$$

(2.19b)

in the whole manifold $A^N$, where $\mu$ runs from 1 to $N$. Without lack of generality, we can choose every member of the set so as to satisfy

$$e_\mu^\nu = \frac{\partial Q_\mu}{\partial q_i} \quad \text{or} \quad dQ_\mu = e_\mu^\nu dq_i,$$

(2.20)

$Q^\mu$, being a function of $q$. The set $\{Q\}$ gives us a new coordinate system, so that we are on the course of rewriting the Langevin equation in terms of the new coordinate system. It is easy to show that we have the orthonormal and completeness conditions

$$e_\mu^\nu e_{\nu i} = \delta_{\mu \nu}, \quad e_\mu^\nu e_{\nu j} = \delta_{ij}$$

(2.21)

for $\{e^\mu\}$ and $\{e_\mu\}$. Then it is obvious that the metric tensor of the new coordinate system is given by

$$g^{\mu \nu} = e_\mu^\nu e_\nu^\nu = \begin{pmatrix} d & 0 \\ 0 & D \end{pmatrix}$$

(2.22a)

or

$$g_{\mu \nu} = e_{\mu i} e_{\nu i} = \begin{pmatrix} d^{-1} & 0 \\ 0 & D^{-1} \end{pmatrix},$$

(2.22b)

which satisfy $g^{\mu \nu} g_{\nu \nu} = \delta_{\mu \nu}$. It is evident that the matrix $(g^{\mu \nu})$ is positive and not singular. In terms of $\{e^\mu\}$ and $\{e_\mu\}$, the projection matrices $P$ and $R$ can be rewritten as

$$P_{ij} = \delta_{ij} - e_\mu^a e_{\mu j},$$

$$R_{ij} = e_\mu^a e_{\mu j},$$

(2.23)

so that we can easily diagonalize them as

$$e_\mu^\nu P_{ij} e_{\nu j} = \delta_{\mu \nu} - \delta_{\mu a} \delta_{\nu a} =$$

$$\begin{pmatrix} 1 \cdots 0 \\ \vdots \ddots \vdots \\ 0 \cdots 1 \end{pmatrix}.$$
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\[ e^i R_{ij} e^{\nu j} = \delta_{\nu a} \delta_{\nu a} = \begin{bmatrix} 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix} \quad (2.24) \]

The same transformation enables us to bring the Langevin equations (2.11a) and (2.11b) into

\[ e^i A q_i = -e^i A \delta S \delta q_i + e^i A \eta_i, \quad (2.25a) \]
\[ e^i A q_i = 0, \quad (2.25b) \]

which immediately become

\[ \dot{Q}^A = -g^{AB} \delta \bar{S} \delta Q^B + e^i A \eta_i, \quad (2.26a) \]
\[ \dot{Q}^a = 0, \quad (2.26b) \]

by virtue of Eq. (2.20), where we have put

\[ \bar{S}(Q^1, \ldots, Q^N) = S(q_1, \ldots, q_N) \quad (2.27) \]

and used the formula

\[ e^i A \delta S \delta q_i = g^{AB} \delta \bar{S} \delta Q^B. \quad (2.28) \]

Equation (2.26b) simply gives the constraints

\[ P^a = Q^a - C^a = 0 \quad (a = N - M + 1, \ldots, N) \quad (2.29) \]

in terms of new coordinates \( \{Q^a\} \), where \( C^a \) is a constant. Consequently, \( \bar{S} \) depends only on random variables \( Q^A \) \( (A = 1, \ldots, N - M) \), so that Eq. (2.26a) is considered to be a Langevin equation for a stochastic process embedded in \( \mathcal{M}^{N-M} \), in other words, on the constraint surface.

Correspondingly to the stochastic process on the constraint surface described by the Langevin equation (2.26a), the well-known prescription gives the Fokker-Planck equation for the scalar probability density \( P \), which is invariant under the general coordinate transformation in \( \mathcal{M}^{N-M} \), as follows:

\[ \dot{P}(Q^A, t) = \frac{1}{\sqrt{g}} \frac{\partial}{\partial Q^A} \sqrt{g} g^{AB} \left[ \frac{\partial}{\partial Q^B} + \delta \bar{S} \bigg|_{Q^a = C^a} \right] P(Q^A, t), \quad (2.30) \]

where \( g = \det g_{AB} \) (see Appendix B). Equation (2.30) has the equilibrium distribution

\[ P_e \propto \exp\left[ -\bar{S}(Q^A, C^a) \right]. \quad (2.31) \]

Taking the metric \( g_{AB} \) of \( \mathcal{M}^{N-M} \) into account, we write down the invariant Fokker-Planck measure as

\[ * \) Note that \( e^i A \delta S \delta q_i \) is a sort of similarity transformation of \( P \).
with respect to the new coordinate system \( \{Q^a\} \), apart from normalization constant. Now we can return to the original coordinate system \( \{q\} \) through the formula

\[
\sqrt{\det g_{AB}} \prod_a^\mu dQ^a = \sqrt{\det g_{AB}} \sqrt{\det g^{ab}} \prod_i dq_i
\]

and then get the final result

\[
d\mu = \exp[-S(q_i)] \prod_a^\mu \delta(F^a) \sqrt{\det g^{ab}} \prod_i dq_i .
\]

This is nothing other than the path-integral measure in Eq. (2·4) obtained on the basis of the canonical formalism.

§ 3. Preliminary discussion toward numerical analyses

We are now discussing stochastic quantization of constrained systems keeping in mind non-perturbative approach to field theory. One of the most powerful methods for the non-perturbative approach is undoubtedly given by numerical analyses. For this purpose, in fact, many authors have been using Monte Carlo calculations to obtain important physical quantities, based on the path-integral representation of the transition amplitude, within the framework of lattice Euclidean field theory. However, if we directly apply the Metropolis method to such path-integral calculations in the case of constrained systems, we shall encounter the following troubles: It is not so easy, in general, i) to generate random variables on the constraint surface, and ii) to calculate practically the determinant factors in the path-integral formula. From this point of view, it would be interesting to examine whether the stochastic quantization method is applicable and useful to the problem, because we can derive correlation functions and then field theoretical propagators via Eq. (1·1), for example, directly from the basic Langevin equation, Eq. (2·9) in the case of constrained systems, irrespectively of the above troubles.

In order to carry out numerical analyses within the framework of the stochastic quantization method, we have to discretize the fictitious time in the basic Langevin equation by replacing Eq. (2·9) with the difference equation:

\[
\ddot{q}_i(t + \Delta t) = q_i(t) + \Delta q_i(t)
\]

with

\[
\Delta q_i(t) = \left[ P_{ij} \left( - \frac{\delta S}{\delta q_j} + \eta_j \right) \right] \Delta t .
\]

Here we have denoted the updated vector (promoted by the discretized Langevin equation) by \( \ddot{q}(t + \Delta t) \) instead of \( q(t + \Delta t) \), because \( \ddot{q}(t + \Delta t) \) steps out of the constraint surface even if \( q(t) \) is kept on the surface. Note that \( \Delta q(t) \) lies on a plane tangential to the constraint surface at \( q(t) \). See Fig. 1. Therefore, successive updating based on the
discretized Langevin equation must destroy
the constraint conditions, so that we should
rectify the above procedure with the help of
additional manipulations for numerical
analyses by the stochastic quantization
method.

Let us consider the 2-dimensional $O(N)$
lattice nonlinear $\sigma$-model whose action and
constraints are given by

\begin{align}
S &= -\frac{1}{2} \beta \sum_{i,j} \sum_{a=1}^{N} J_{ij} \sigma_i^a \sigma_j^a, \\
F_i &= \sum_{a=1}^{N} (\sigma_i^a)^2 -1 = 0,
\end{align}

respectively, where $J_{ij}=1$ for a nearest-neighbouring pair $(i,j)$ and otherwise $J_{ij}=0$, and
$\beta$ is a positive constant. Note that $\sigma_i^a$ stands for the $a$-th component of $O(N)$ spin vector
at the $i$-th site. In this case Eq. (3·1) becomes

\begin{align}
\tilde{\sigma}_i^a(t+\Delta t) &= \sigma_i^a(t) + \Delta \sigma_i^a(t), \\
\Delta \sigma_i^a(t) &= [\beta \sum_b (\delta^{ab} - \delta_i^a (t) \sigma_i^b(t)) (\sum_{j} J_{ij} \sigma_j^b(t) + \eta_i^b(t))] \Delta t,
\end{align}

which gives, of course, an updating process to destroy the constraint condition. An
ttempt to rectify the procedure is made through a sort of renormalization

\begin{equation}
\sigma_i^a(t+\Delta t) = \frac{\tilde{\sigma}_i^a(t+\Delta t)}{\sqrt{\sum_{a=1}^{N} \tilde{\sigma}_i^a(t+\Delta t) \tilde{\sigma}_i^a(t+\Delta t)}}
\end{equation}

by hand. It seems that the renormalization method does not necessarily yield nice
results for correlation functions, which are not in good agreement with values given by
the Metropolis method especially for small $N$. Apart from discussion on numerical
results, however, we have to raise a general question about such an artificial renormaliza­
tion because it must spoil the basic Langevin equation.

A possible way of improving the above situation may be to replace the time-by-time
constraints with more moderate ones. Really, we can say, the time-by-time constraints
are too strong to the stochastic quantization method, because we have only to reproduce
the ordinary field theory only at the infinite fictitious time limit in our scheme. In the next
section, we propose to use new types of constraints different from the time-by-time
constraints within the framework of the stochastic quantization method.

§ 4. New types of constraints

Here we propose new types of constraints: (i) converging constraints and (ii) fluctuat­
ing constraints, which are more moderate than the time-by-time constraints.
4.1. Converging constraints

Our first proposal is to replace the Langevin equation (2·6a) under the time-by-time constraints Eq. (2·6b) or Eq. (2·7) with the following set of equations:

\[ \dot{q}_i = -\left( \frac{\partial S}{\partial q_i} + \lambda^a \frac{\partial F^a}{\partial q_i} \right) + \eta_i, \quad (i = 1, \ldots, N) \]  
\[ F^a = -\chi F^a, \quad (a = N - M + 1, \ldots, N) \]

where \( \chi \) is an arbitrary positive constant with dimension of \( t^{-1} \) to be adjusted in numerical analyses. We may call Eq. (4·1b) converging constraints in the sense that they will converge to \( F^a = 0 \) as \( t \to \infty \). Hence we have

\[ \frac{\partial F^a}{\partial q_i} \dot{q}_i = -\chi F^a \quad (a = N - M + 1, \ldots, N) \]

instead of Eq. (2·7) in the case of the time-by-time constraints. In spite of the modification of constraints, it is evident that we have the same equilibrium distribution as Eq. (2·4) or Eq. (2·34) because \( \lim_{t \to \infty} F(a(q(t)) = 0 \). Using Eqs. (4·1a) and (4·2), we can eliminate the Lagrange multipliers \( \lambda^a \)'s to obtain

\[ \dot{q}_i = P_{ij} \left( -\frac{\partial S}{\partial q_j} + \eta_j \right) - \chi \frac{\partial F^a}{\partial q_i} (D^{-1})^{ab} F^b, \]

where \( P \) and \( D \) are defined by Eqs. (2·10) and (2·5), respectively. The last term on the r.h.s. of Eq. (4·3) is a new constraint force, generated from the converging constraints, which is perpendicular to the constraint surface \( \mathcal{M}^{N-M} \) given in §2 as is easily shown. The new constraint force may be called restoring force, because it works toward the constraint surface, as is schematically shown by Fig. 2, only when the dynamical configuration steps out of \( \mathcal{M}^{N-M} \). The converging constraints are suggested by the same ones developed by Yamashita \( ^8 \) and Tanabe \( ^9 \) in the theory of optimization. The present method can be expected to work also in stochastic quantization method as well as in the theory of optimization. As mentioned in §3, the Langevin equation discretized for numerical analyses kicks, in general, updated vector out of the constraint surface \( (F^a = 0) \), so that the restoring force plays an important role there to pull them back toward the surface. For the sake of practical convenience for numerical analyses, it is rather better to regard \( \chi \) as a positive function of \( F^a \) (consequently, of \( q \)), by which we shall also be led to the original constraints \( F^a = 0 \) as \( t \to \infty \), for the following reason: \( \chi \) can be so adjusted as to revive \( F^a(q(t+2n\Delta t)) = 0 \) (\( n \) being an integer) by every two (or generally, a few) updating steps starting from a vector, i.e., \( q(t) \), on the constraint surface. Needless to say, we have only to pick up vectors, \( q(t+2n\Delta t) \), on the constraint surface, in order to calculate physical quan-
tities. In fact, we shall see that the present method improves numerical analyses of the lattice $O(N)$ nonlinear $\sigma$-model rather than the original one based on the time-by-time constraints, as will be reported in another paper\textsuperscript{7} by Rikihisa, Tanaka and ourselves.

4.2. Fluctuating constraints

Another modification of constraints also comes from the ‘penalty function method’ in the theory of optimization. Following the idea, we have to start with the Langevin equation

$$\dot{q}_i = -\left( \frac{\delta S}{\delta q_i} + \lambda^a \frac{\partial F^a}{\partial q_i} + \varepsilon^a F^a \frac{\partial F^a}{\partial q_i} \right) + \eta_i. \quad (4.4)$$

Here, $\varepsilon^a$ and $\lambda^a$ are free parameters which are so adjusted later as to give the conditions:

$$\lim_{t\to\infty} \langle F^a(q) \rangle = 0, \quad (a = N - M + 1, \ldots, N) \quad (4.5a)$$

and

$$\lim_{t\to\infty} \langle (F^a(q))^2 \rangle = 0. \quad (4.5b)$$

The conditions may not necessarily be regarded as constraints in the exact terminology, but work to revive the original constraints $F^a = 0$ as $t\to\infty$, as will be seen shortly. Equation (4.4) with finite $\lambda^a$ and $\varepsilon^a$ yields the equilibrium distribution

$$P_b(q) \propto \exp \left[ -\left( S + \int dx \left( \lambda^a F^a + \frac{1}{2} \varepsilon^a (F^a)^2 \right) \right) \right] \quad (4.6)$$

at the limit $t\to\infty$. We have to keep all $\varepsilon^a$'s positive to use the formula

$$\lim_{\varepsilon^a \to 0} \frac{\varepsilon^a}{2\pi} e^{-\varepsilon^a/2} \delta(F^a) = \delta(F^a), \quad (4.7)$$

which will produce a factor $\delta(F^a)$ in $P_b(q)$ and equivalently, give Eq. (4.5) at the limit $\varepsilon^a \to \infty$. However, we must work with finite (but large) $\varepsilon^a$'s in numerical analyses — in this case $F^a$ fluctuates around $-\lambda^a/\varepsilon^a \approx 0$. This is the reason why we call Eq. (4.4) with Eq. (4.5) the Langevin equation under fluctuating constraints.

Applying $P$ and $R$ (defined by Eq. (2.10)) to Eq. (4.4) and making use of a new time $\tau = \varepsilon t$, $\varepsilon$ being a positive constant with dimension of $t^{-1}$, we obtain

$$P_{ij} \frac{dq_j(\tau)}{d\tau} = -\frac{1}{\varepsilon} P_{ij} \frac{\delta S}{\delta q_j} - \frac{1}{\sqrt{\varepsilon}} P_{ij} \xi_j(\tau), \quad (4.8a)$$

$$R_{ij} \frac{dq_j(\tau)}{d\tau} = -\varepsilon^a F^a \frac{\partial F^a}{\partial q_i} - \frac{1}{\varepsilon} \left( R_{ij} \frac{\delta S}{\delta q_j} + \lambda^a \frac{\partial F^a}{\partial q_j} \right) + \frac{1}{\sqrt{\varepsilon}} R_{ij} \xi_j(\tau). \quad (4.8b)$$

Here we have put $\varepsilon^a = \varepsilon \varepsilon^a$ and

$$\xi_j(\tau) = -\frac{1}{\sqrt{\varepsilon}} \eta_i(t) \quad (4.9a)$$

with statistical properties

$$\langle \xi_i(\tau) \xi_j(\tau') \rangle = 2\delta_{ij} \delta(\tau - \tau'), \quad (4.9b)$$
which means that $\xi(t)$'s are random forces independent of $\epsilon$. It is easily shown that, in Eq. (4·8), the systematic forces with $\epsilon^{-1}$ are of the same order of magnitude as $\xi(t)/\sqrt{\epsilon}$ with respect to $\epsilon$. Hence we can safely discard the second and third terms on the r.h.s. of Eq. (4·8b) leaving the first term as $\epsilon \to \infty$ keeping $\epsilon^a$ finite, so that we have

$$R_{ij} \frac{dq_j(t)}{d\tau} = - \epsilon^a F^a \frac{\partial F^a}{\partial q_i}$$

(4·10)

instead of Eq. (4·8b). Equation (4·10) implies that perpendicular components of the random forces do not work for very large $\epsilon$. As a result, Eq. (4·4) can safely be replaced with

$$\dot{q}_i = - \left( \frac{\delta S}{\delta q_i} + \lambda^a \frac{\partial F^a}{\partial q_i} + \epsilon^a F^a \frac{\partial F^a}{\partial q_i} \right) \hat{P}_j \eta_j$$

(4·11)

for very large $\epsilon$.

Equation (4·10) is easily reduced to

$$\frac{dF^a}{d\tau} = - D^{ab}(\epsilon^b F^b),$$

(4·12)

which also revives the original constraints, $F^a = 0$, as $\tau \to \infty$ because of the positiveness of matrix $(D^{ab})$. The Langevin equation (4·8a) on the constraint surface simply gives the equilibrium distribution in $\mathcal{M}^{N-M}$ proportional to $\exp[-\tilde{S}(Q^a, C^a)]$, so that we are led to Eq. (2·4) or Eq. (2·34) through the same route as in the case of §2 or §3.

Finally we discuss a somewhat similar but different method suggested by Guha and Lee,\(^{10}\) which is based on Eq. (4·4) with $\epsilon^a = 0$ together with Eq. (4·5a) alone. Note that they have never required Eq. (4·5b). It is important to remark that we cannot obtain the exact result Eq. (2·4) or Eq. (2·34), generally speaking, with lack of Eq. (4·5b). To compare the present method with Guha and Lee's one, let us consider a simple static model whose action is given by

$$S = \frac{1}{2}(x^2 + y^2)$$

(4·13)

under a constraint

$$F = x + y - 1 = 0.$$  

(4·14)

This model is nothing but static statistical mechanics of a particle in a potential given by the bold curve shown in Fig. 3. We can immediately obtain

$$\langle x \rangle = \langle y \rangle = \frac{1}{2}, \quad \langle x^2 \rangle = \langle y^2 \rangle = \frac{3}{4},$$

(4·15)

using the formula...
\[ \langle f \rangle = \iint f(x, y) e^{-s(x + y - 1)} dx dy / \iint e^{-s(x + y - 1)} dx dy \]

for average of \( f(x, y) \). Note that \( \det(D) = 1 \) in this case. Now we try to apply the present method to this model. Given the action Eq. (4-13), Eq. (4·4) is written as

\[
\begin{align*}
\dot{x} &= -(x + \lambda + \epsilon(x + y - 1)) + \eta_x , \\
\dot{y} &= -(y + \lambda + \epsilon(x + y - 1)) + \eta_y ,
\end{align*}
\]

which are exactly solved to give

\[
\begin{align*}
\langle x \rangle &= \langle y \rangle = (\epsilon - \lambda)/(2\epsilon + 1) , \\
\langle x^2 \rangle &= \langle y^2 \rangle = (3\epsilon^2 - 3\epsilon - 2\epsilon\lambda + \lambda^2 + 1)/(2\epsilon + 1)^2 .
\end{align*}
\]

By making use of the exact solution, conditions (4·5a) and (4·5b) are explicitly expressed as

\[
\begin{align*}
\lim_{t \to \infty} \langle F \rangle &= -\frac{2\lambda + 1}{2\epsilon + 1} = 0 , \\
\lim_{t \to \infty} \langle F^2 \rangle &= \frac{2}{2\epsilon + 1} + \left( \frac{2\lambda + 1}{2\epsilon + 1} \right)^2 = 0
\end{align*}
\]

in terms of \( \lambda \) and \( \epsilon \). We have to take the limit \( \epsilon \to \infty \) in order that the equilibrium distribution (4·6) gives \( \delta(x + y - 1) \) in this case. Consequently, both conditions (4·18a) and (4·18b) exactly hold with arbitrary \( \lambda \) at the limit \( \epsilon \to \infty \), and then Eq. (4·17) gives the same results as Eq. (4·15).

On the other hand, if we keep \( \epsilon \) finite, for example, \( \epsilon = 0 \) as in the Guha-Lee case, Eq. (4·18b) never holds exactly even though Eq. (4·18a) is satisfied by \( \lambda = -1/2 \). It is true that Guha and Lee have not required Eq. (4·5b) and then (4·18b) to be satisfied, but we are left having \( \langle x \rangle = \langle y \rangle = 1/2 \) and \( \langle x^2 \rangle = \langle y^2 \rangle = 5/4 \) not in agreement with the exact results Eq. (4·15). Consequently, we conclude that both Eqs. (4·5a) and (4·5b) should be required.

§ 5. Concluding remarks

In this paper we have formulated the stochastic quantization method to be applied to constrained systems by introducing the three types of constraints, (i) time-by-time constraints, (ii) converging constraints and (iii) fluctuating constraints, which are to be imposed on the basic Langevin equation. We have first shown that the present method really produces the same measure as given by the path-integral quantization. Furthermore it has been stressed that the latter two types of constraints will serve to make numerical analyses feasible when applied to a dynamical system with nonlinear constraints. Detailed discussions on numerical analyses will be reported in a separate paper.}

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Appendix A

— Derivation of Lagrangian Path-Integral Formula —

Here we derive Eq. (2.4) from Eq. (2.3). The canonical momenta in Eq. (2.3) are defined by

\[ p_i = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial \dot{x}_0}, \quad (i = 1, \ldots, N) \] (A.1)

\[ \pi_a = \frac{\partial L}{\partial \dot{\lambda}_a} = 0, \quad (a = 1, \ldots, M) \] (A.2)

in which Eq. (A.2) should be regarded as primary constraints

\[ \Omega_1^a = \pi_a \approx 0, \] (A.3)

where \( \approx \) represents the weak equality. The canonical Hamiltonian is then given by

\[ \tilde{H}(p, \pi, q, \lambda) = H + \lambda_a F^a, \] (A.4)

where \( H \) is Hamiltonian corresponding to \( L \) without constraints, i.e.,

\[ H(p, q) = p_i \frac{dq_i}{dx_0} - L. \] (A.5)

Then we have the total Hamiltonian:

\[ H_T(p, \pi, q, \lambda) = H + \lambda_a F^a + w_a \pi_a. \] (A.6)

The arbitrary function \( w_a \) is to be determined later.

The primary constraints (A.3) must always hold with respect to real time \( x_0 \), so that we must require to have \( \{ \Omega_1^a, H_T \} = 0 \). The requirement generates new constraints to be called the secondary constraints. This procedure must be repeated until new independent constraints are no more produced. For Hamiltonian (A.6) we list up all the secondary constraints as follows:

\[ \Omega_2^a = F^a \approx 0, \] (A.7)

\[ \Omega_3^a = \frac{\partial F^a}{\partial q_i} \frac{\partial H}{\partial p_i} \approx 0, \] (A.8)

\[ \Omega_4^a = G^a - C_i^{ab} \lambda_b \approx 0, \] (A.9)

where

\[ G^a(p, q) = \{ \Omega_2^a, H \}, \] (A.10)

\[ C_i^{ab}(p, q) = \frac{\partial F^a}{\partial q_i} \frac{\partial^2 H}{\partial p_i \partial q_j} \frac{\partial F^b}{\partial q_j}. \] (A.11)

Let us assume \( \det C_i^{ab} \neq 0 \), then we can determine the arbitrary function \( w_a \) as

\[ w_a = (C_i^{-1})^{ab} \left[ \{ G^b, H \} - \left( \frac{\partial G^b}{\partial p_i} \frac{\partial G^c}{\partial q_i} + \{ C_i^{bc}, H \} - \frac{\partial C_i^{bc}}{\partial q_i} \frac{\partial F^d}{\partial q_i} \lambda_d \right) \lambda_c \right]. \] (A.12)
using the consistency conditions \(\{Q_i^a, H_T\} = 0\) at the last step of the above procedure. All the sets of constraints (A·3), (A·7), (A·8) and (A·9) belong to the 'second class' characterized by

\[
\begin{align*}
\{Q_1, Q_1^b\} &= 0, \quad \{Q_2, Q_2^b\} = 0, \quad \{Q_3, Q_3^b\} = 0, \quad \{Q_4, Q_4^b\} = C_1^{ab}, \\
\{Q_2, Q_2^b\} &= C_1^{ab}, \quad \{Q_5, Q_5^b\} = C_2^{ab}, \\
\{Q_3, Q_3^b\} &= C_3^{ab}, \quad \{Q_4, Q_4^b\} = C_4^{ab}, \\
\{Q_4, Q_4^b\} &= C_5^{ab}.
\end{align*}
\]

Note that we need not have the explicit forms of \(C_2^{ab}, C_3^{ab}, C_4^{ab}\) and \(C_5^{ab}\) in order to obtain the path-integral measure. For the \((4M) \times (4M)\) matrix \(\{Q_{ab}, Q_{ba}\}\) \((a, b = 1, \ldots, M; \alpha, \beta = 1, 2, 3, 4)\), we rearrange elements in its determinant in the form

\[
\begin{bmatrix}
\{Q_1^a, Q_1^b\} & \{Q_1^a, Q_2^b\} & \{Q_1^a, Q_3^b\} & \{Q_1^a, Q_4^b\} \\
\{Q_2^a, Q_1^b\} & \{Q_2^a, Q_2^b\} & \{Q_2^a, Q_3^b\} & \{Q_2^a, Q_4^b\} \\
\{Q_3^a, Q_1^b\} & \{Q_3^a, Q_2^b\} & \{Q_3^a, Q_3^b\} & \{Q_3^a, Q_4^b\} \\
\{Q_4^a, Q_1^b\} & \{Q_4^a, Q_2^b\} & \{Q_4^a, Q_3^b\} & \{Q_4^a, Q_4^b\}
\end{bmatrix}
\]

\[
= \det \begin{pmatrix}
C_1^{ab} & 0 & 0 & 0 \\
C_2^{ab} & C_1^{ab} & 0 & 0 \\
C_3^{ab} & C_2^{ab} & -C_1^{ab} & 0 \\
C_4^{ab} & C_3^{ab} & -C_2^{ab} & -C_1^{ab}
\end{pmatrix}
\]

\[
= (\det C_i^{ab})^4.
\]

Consequently, the path-integral formula (2·3) can be rewritten in the following way:

\[
\langle f | i \rangle = \int \prod_{\alpha=1}^{4M} \delta(\pi_a) \delta(F^a) \delta\left(\frac{\partial F^a}{\partial \pi_i} \frac{\partial H}{\partial \phi_i}\right) \delta(G^a - C_i^{ab} \lambda_b) (\det C_i^{ab})^2
\]

\[
\times \exp\left[i \int dx_0 \left(\frac{d\pi_i}{dx_0} + \pi_a \frac{d\lambda_a}{dx_0} - H - \lambda_a F^a - \omega_a \pi_a\right)\right]
\]

\[
\times \prod \frac{dp_i dq_i}{2\pi} \exp\left[i \int dx_0 \left(\frac{d\pi_i}{dx_0} - H\right)\right].
\]

We have obtained the last line by integration over \(\pi^a\) and \(\lambda^a\).

For simplicity we assume that matrix \((\partial^2 H/\partial \phi_i \partial \phi_j)\) does not depend on \(q\) and is positive, as in most cases of conventional field theories. Then after an appropriate transformation, we can express \(H\) in a diagonal form, that is,
In this case $C_{ab}$ becomes $D_{ab}$. Now we come to the place to obtain the final expression by integration over $p$ and $\rho$:

$$H = \frac{1}{2} \sum_i p_i^2 + V(q).$$  \hspace{1cm} (A\cdot16)

Going to Euclidean space, we get the Lagrangian path-integral formula Eq. (2-4).

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**Appendix B**

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**Derivation of Fokker-Planck Equation**

We derive here the Fokker-Planck equation (2-30) from the Langevin equation (2-26) along the line of thought given by our previous works.\(^{(1)}\) By making use of distorted random forces defined by

$$\eta^a = e_i^a \eta_i , \quad \eta^a = e_i^a \eta_i$$  \hspace{1cm} (B\cdot1)

and relations

$$\eta_i \eta_t = \eta^a g_{ab} \eta^b + \eta^A g_{AB} \eta^B,$$

$$\prod_i d\eta_i = \sqrt{\det g_{ab}} \prod_a d\eta^a \sqrt{\det g_{AB}} \prod_A d\eta^A,$$  \hspace{1cm} (B\cdot2)\(^*\)

the Gaussian distribution $\exp[-(1/4)\eta_i \eta_t \prod_i d\eta_i]$ with respect to $\eta_i$'s can be replaced by

$$e^{-(1/4)\eta^a g_{ab} \eta^b} \sqrt{\det g_{AB}} \prod_A d\eta^A$$  \hspace{1cm} (B\cdot3)

with respect to $\eta^A$'s, where we have discarded the $\eta^a$-distribution because the Langevin equation (2-26) never depends on $\eta^a$'s. From Eq. (B\cdot3), taking the Markovian nature into account, one can derive the Gaussian distribution for $Z^A = \int_t^{t+\Delta t} \eta^A(t) dt$ as follows:

$$e^{-(1/4\Delta t)\eta^a g_{ab} \eta^b} \sqrt{\det g_{ab} / \Delta t} \prod_A d\eta^A,$$  \hspace{1cm} (B\cdot4)

which means the joint probability of finding process $(Q^A, t - \Delta t) \rightarrow (Q^A, t)$ if we replace $Z^A$'s with $Q^A$'s given by the Langevin equation.

\(^*\) Note that fundamental vectors $e_i^a(q(t))$ and $e_i^a(q(t))$ do not depend on $\eta_i(t)$'s but only on $\eta_i(t')$'s for $t' < t$, because the Langevin equation as a stochastic differential equation means that $q_i(t)$ is independent of $\eta_i(t)$'s.
Consequently, the Kolmogoroff-Chapman equation, infinitely repeated with Eq. (B·5), gives the path-integral representation

\[ P(Q^A, t|Q'^A, t') = \int \sqrt{\text{det} g_{AB}} \prod_A dQ^A \times \exp \left[ -\frac{1}{4} \int_{t'}^{t} dt'' \left( Q^A + g^{AC} \frac{\delta S}{\delta Q^C} \bigg|_{Q^a=\text{c}a} \right) g_{AB} \left( Q^B + g^{BD} \frac{\delta S}{\delta Q^D} \bigg|_{Q^a=\text{c}a} \right) \right] \]  

for the joint probability from \((Q'^A, t')\) to \((Q^A, t)\), apart from the normalization constant. Note that \(\text{det}(\partial S'/\partial Q^B) = 1\). From Eq. (B·6) we can easily derive the following invariant Fokker-Planck operator:

\[ H_{FP} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial Q^A} \sqrt{g} g^{AB} \left[ \frac{\partial}{\partial Q^B} + \frac{\delta S}{\delta Q^B} \bigg|_{Q^a=\text{c}a} \right] \]  

appearing in Eq. (2·30). Detailed discussions will be given in a forthcoming paper.

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