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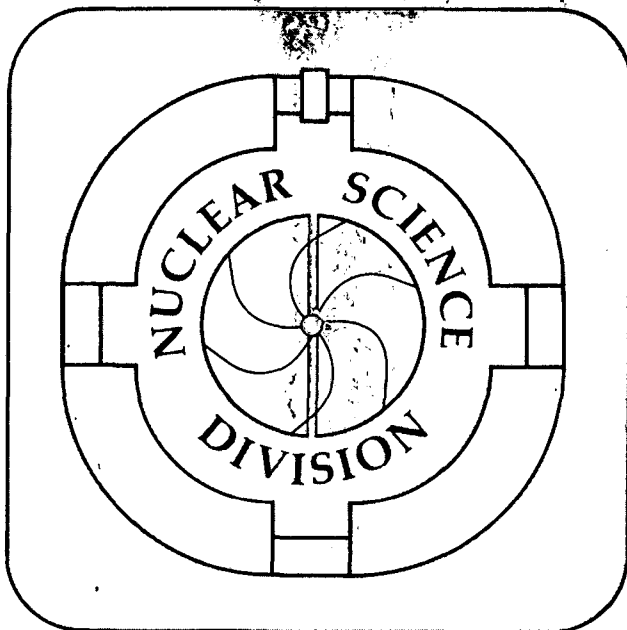
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MICROCANONICAL QUANTIZATION AND ITS APPLICATIONS*

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ABSTRACT

We discuss microcanonical quantization and its interesting properties and explain our recent proposal for a numerical application.

Microcanonical quantization[1,2] is derived from the analogy between statistical mechanics and functional quantization of fields. As is well-known, the standard functional quantization in Euclidean space may be recognized as classical canonical ensemble averages. With the Euclidean action $S_0(\phi)$ of a field ϕ, the functional quantization leads to

$$\langle f(\phi) \rangle = \frac{1}{Z_0} \int D\phi \, f(\phi) e^{-S_0(\phi)} \quad , \quad Z_0 \equiv \int D\phi \, e^{-S_0(\phi)} \tag{1}$$

where $f(\phi)$ is a physical quantity. This equation may be rewritten by inserting auxiliary variables, P_i

$$\langle f(\phi)\rangle = \frac{1}{Z} \int DPD\phi \; f(\phi)e^{-\beta H(P,\phi)} \quad , \quad Z \equiv \int DPD\phi \, e^{-\beta H(P,\phi)}$$

$$H \equiv \sum_{i=1}^{N} \frac{P_i^2}{2} + \frac{S_0(\phi)}{\beta} \qquad\qquad (2)$$

where β is an arbitrary constant and the index i runs over the dynamical degrees of freedom of the field ϕ (e.g. lattice sites if we adopt the lattice regularization). The equation (2) gives the canonical ensemble average in a system with Hamiltonian $H(P,\phi)$ and a temperature β^{-1}; P_i and ϕ_i are canonical conjugates to each other. We thus understand that functional quantization is equivalent to taking the canonical ensemble average. Then, we are led naturally to introduce a microcanonical ensemble $\delta(E - H)$ and to take an average as

$$\langle f(\phi)\rangle_m = \frac{1}{Z_m} \int DPD\phi \; f(\phi)\delta(E - H) \quad , \quad Z_m \equiv \int DPD\phi \; \delta(E - H) \quad .$$

$$(3)$$

This is just the one as we call microcanonical quantization.[1] This method has been used[3] numerically in lattice gauge theories and the numerical results agree well with Monte-Carlo results of (1).

To formulate the method more rigorously, we need to take a regularization (hereafter, we use the lattice regularization) and to take a finite volume (=V). The equivalence between $\langle f\rangle$ and $\langle f\rangle_m$ has been proved[1]

perturbatively in the limit of the infinite volume,

$$\lim_{V \to \infty} <f> = \lim_{V \to \infty} <f>_m \qquad (4)$$

In this proof of the perturbative equivalence, the energy in eq. (3) should be taken as $E = N/\beta$, where N is the number of dynamical degrees of freedom ($DPD\phi \equiv \sum_{i=1}^{N} dP_i d\phi_i$). It goes without saying that perturbation theory is reliable in the limit of small coupling constant, g. Hence, the relation of $E = N/\beta$ holds only around $g = 0$. To show the equivalence in eq. (4) for arbitrary g, it can be argued that we need the following relation,

$$E = \frac{N}{2\beta} + \frac{1}{Z_0} \int D\phi \; e^{-S_0} S_0/\beta \qquad (5)$$

where $N/2\beta$ comes from the kinetic energy of $\sum_{i=1}^{N} P_i^2/2$. The origin of this relation is easy to understand by taking the canonical average of $H(P,\phi)$. In addition, we need some further assumptions in the proof of the equivalence for general g, which are physically reasonable and rather weak, see ref. 1. The eq. (5) may be replaced with

$$E = \frac{N}{2\beta} + \frac{1}{\beta} <S_0>_m \qquad (6)$$

This is a consistency condition, which is useful in numerical calculations.

In short, the microcanonical quantization is performed by use of the microcanonical ensemble and with the consistency

condition in eq. (6). We can check explicitly its validity by examining several solvable problems in the statistical mechanics. For example, we have computed the magnetizations in a classical Heisenberg spin model by use of a mean field approximation. That calculation is a bit tedious and we need some tricks, even though that problem can be solved simply in the canonical ensemble average.

Now, we comment on some interesting features of the microcanonical quantization. One of them is the absolute convergence of a perturbation series,[4] which is defined by expanding $\delta(E - H)$ with respect to the coupling constant g by regarding E as an independent constant: We are considering a situation where the action S_0 has a form as $S_0 = S_f + gS_I$ (scalar field theory) or $S_0 = S/g^2$ (lattice gauge theory). Hence, eq. (6) is used to determine E in terms of g after we sum the perturbation series of $\langle S \rangle_m$. It is amazing that, by using this perturbation theory, we can obtain, in principle, not only asymptotic properties as $g \to 0$, but also general properties for arbitrary g of the quantum field theory. We note that the standard perturbation series in the functional quantization does not converge even if the theory has ultraviolet and infrared cutoffs; this implies that the standard perturbation theory reveals only asymptotic properties of the theory as $g \to 0$.

Another interesting feature lies in its numerical applications[3,5] where one postulates the "ergodicity" of the energy surface $E = H$ in phase space $\{P_i, \phi_i\}$. We shall consider a U(1) lattice gauge theory as an example. The

action of the lattice gauge theory is a function of the link variables, $U_i = e^{i\theta_i}$ and the inversed coupling constant, β: $S_0 = \beta S(U)$. If we identify β in eq. (2) with this inversed coupling constant, the Hamiltonian becomes $H = \sum_{i=1}^{N} P_i^2/2 + S(U)$ and the microcanonical ensemble average is given by

$$\langle f \rangle_m = \frac{1}{Z_m} \int \prod_{i=1}^{N} dP_i \, d\theta_i \, \delta(E - H) f(\theta) \quad , \quad 2\pi \geq \theta \geq 0 \quad . \quad (7)$$

We note that $N/2\beta$ can be computed as

$$\frac{N}{2\beta} = \left\langle \sum_{i=1}^{N} P_i^2/2 \right\rangle_m \quad (8)$$

This means that each kinetic energy contributes $1/2\beta$ to the energy (equipartition law); β^{-1} plays the role of temperature.

Now, let us assume ergodicity of the classical system described by the Hamiltonian $H(P,\theta)$. This assumption allows us to compute $\langle f \rangle_m$ by solving the Hamliton's equations,

$$\frac{d\theta_i}{d\tau} = \frac{\partial H}{\partial P_i} \quad , \quad \text{and} \quad \frac{dP_i}{d\tau} = -\frac{\partial H}{\partial \theta_i} \quad (9.a)$$

and by taking an average over time τ,

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T f(\theta(\tau)) dz = \langle f \rangle_m \quad . \quad (9.b)$$

The ergodicity is expected to hold in almost all nonlinear systems for sufficiently large number of the dynamical degrees of freedom. Therefore, in the microcanonical quantization, problems in the quantum theory are reduced to problems in the

corresponding classical theory. However, if the system has some explicit symmetries, the ergodicity doesn't hold. In our case of the U(1) lattice gauge theory, we have local gauge symmetries, which allow us to reduce some irrelevant cyclic variables. Hence, in order to apply the above procedure, we must reformulate the microcanonical quantization in terms of independent dynamical variables. This leads us to solve the Hamilton's equation for all variables (θ, P) under initial conditions such as $P_i = 0$ for all i. Then, the irrelevant variables P_i' vanish at any time so that we must replace N in the left hand side of eq. (8) with the number of independent degrees of freedom, N_{in}. As an example, we have performed the numerical calculation of $<S>_m$ vs β using this method. We adopt a lattice size of 4^4 and S as

$$S = \sum_p (1 - \frac{1}{2}(U_p + U_p^+)) \quad , \quad U_p \equiv \sum_{i \in p} e^{i\theta_i} \qquad (10)$$

where P indicates a plaquette.

First, we start with random configuration of θ_i and with $P_i = 0$ for all i, and thermalize the system. The temperature β^{-1} and the internal energy $<S>_m$ are measured by taking their averages over large enough time interval T,

$$\frac{N_{in}}{2\beta} = \frac{1}{T} \int_0^T \sum_{i=1}^N P_i^2/2 \, d\tau \quad \text{and} \quad <S>_m = \frac{1}{T} \int_0^T S(\theta(\tau)) d\tau \quad , \qquad (11)$$

where $\tau = 0$ is not the initial time, but a time after the system is thermalized. Next, we decrease (or increase) the temperature. To do so, we use our recently proposed method[5]

for changing the temperature. That is, we put a friction term into the Hamilton's equations

$$\frac{d\theta_i}{d\tau} = \frac{\partial H}{\partial P_i} \quad \text{and} \quad \frac{dP_i}{d\tau} = -\frac{\partial H}{\partial \theta_i} + c'P_i \tag{12}$$

with $c' \equiv C_0 / \sum_{i=1}^{N} P_i^2$, where C_0 is a constant (hereafter, we only discuss the case of decreasing the temperature, that is, $C_0 > 0$). Due to this friction term, the energy of the system decreases as $\frac{dH}{d\tau} = -C_0$, and the temperature also decreases continuously in time. Hence, if we measure β and $\langle S \rangle_m$ as a function of the time, τ, we can determine the relation between β and $\langle S \rangle_m$. We depict the result in Fig. 1, which agree well with Monte-Carlo results. We conclude that the microcanonical simulation described above works well.

Fig. 1.

N_p = # of plaquette

C_0 = 2

T = 2500
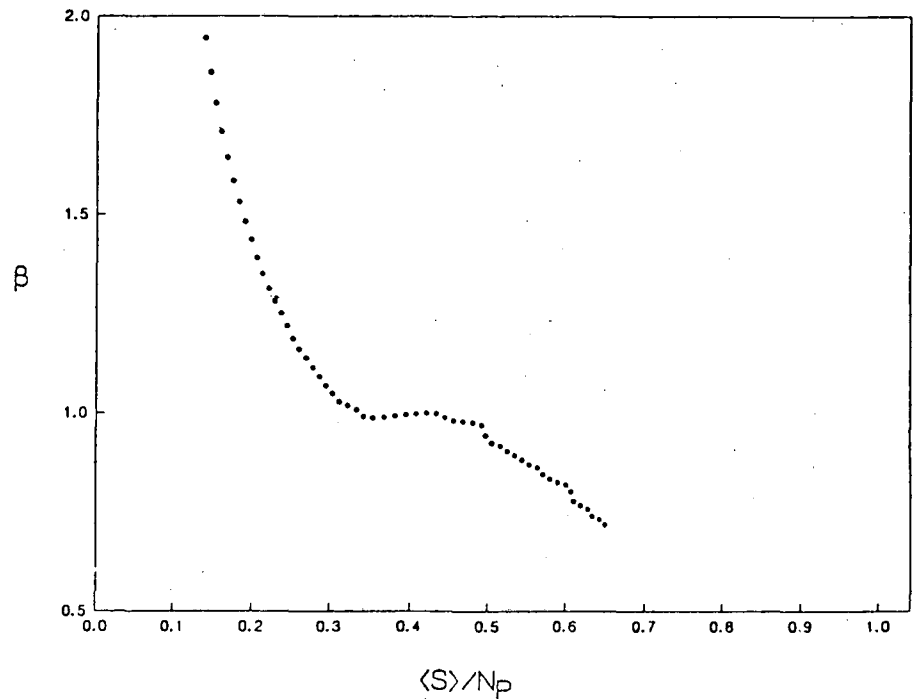
As a final comment on an interesting feature of the microcanonical simulation, we shall briefly state an application of our proposal to identify the order of phase

transitions. The distinction of first order phase transitions with second order ones has been performed mainly in Monte-Carlo simulations by examining, for example, the continuity of the internal energy. However, the discontinuity of a critical point of the first order is smoothed out by finite volume effects. On the other hand, it is possible in the microcanonical simulation to identify the first order phase transitions even in a finite volume.

According to the microcanonical simulation, we can find the internal energy of supercooled (or superheated) metastable states. Namely, for a system with sufficiently small volume, its internal energy $<S>_m$ becomes a multi-valued function of the temperature β^{-1} beyond a critical point of a first order. One branch of the function corresponds to the energy of the supercooled (or superheated) state. This is because, even beyond the critical point, such metastable states cannot decay into a stable state; surface energy effects between the two phases prevent the decay of the metastable states in a system with sufficiently small volume. The multi-valuedness is revealed by examining the so-called S shaped curve[6] in the $<S>_m$ vs. β plane. On the other hand, the multi-valuedness is not expected around a critical point of second order. The reason is that the internal energy is smooth at this critical point.

Taking an action,

$$S = \sum_p \left\{ (1 - \frac{1}{2} (U_p + U_p^+)) + (1 - \frac{1}{2} (U_p^2 + U_p^{+2})) \right\} \tag{13}$$

we depict these typical S shaped curves in Fig. 2 which was obtained by using our method[5] in eq. (12) for decreasing the temperature; curve B is from ref. 6 where a different method for decreasing the temperature was used in the microcanonical simulation. Curves A and C correspond to different choices of the parameter C_0. The reason for a difference between these two curves around the critical point is that the extent to which the system is supercooled depends on the rate $(=C_0)$ at which the temperature is decreased. We find that our curves, A and C, show more clearly S shape behavior of the system than does the curve B obtained by another method. Therefore, it is possible to obtain fairly clear S shaped curves by choosing an appropriate friction coefficient, C_0, and hence to identify unambiguously the first order phase transition.

Fig. 2.

A:

C_0 = 10

T = 2000

B:

C_0 = 5

T = 4000
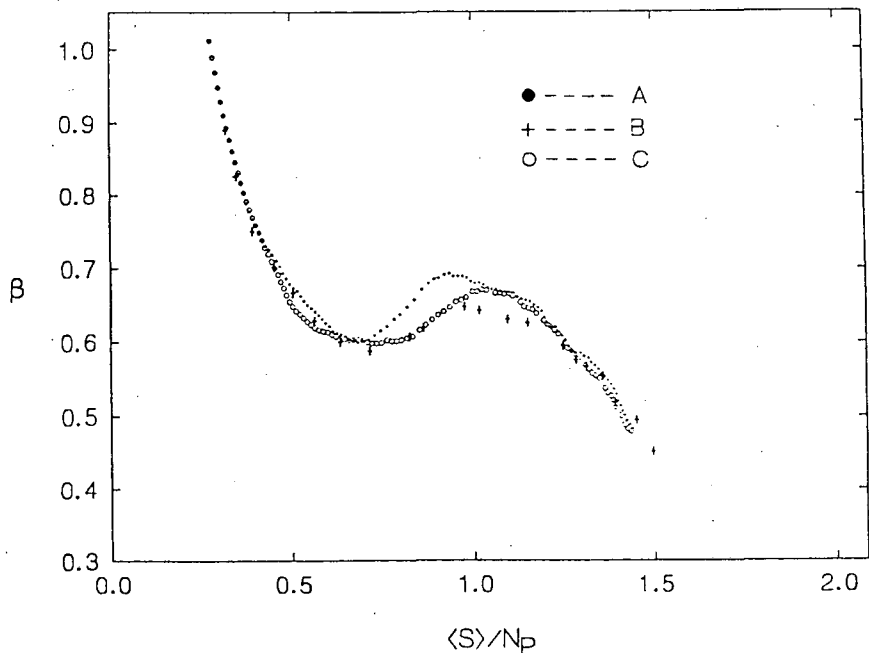
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REFERENCES

1. A. Iwazaki, Phys. Lett. 141B (1984) 342, LBL preprint LBL-19909 to be published in Phys. Rev. D.

2. D.J.E. Callaway and A. Rahman, Phys.Rev. Lett. 49 (1982).

3. M. Creutz, Phys. Rev. Lett. 50 (1983) 1411.
   J. Polony and H.W. Wyld, Phys. Rev. Lett. 51 (1983) 2257.
   J. Polony, H.W. Wyld, J.B. Kogut, J. Shigemitsu and D.K. Sinclair, Phys. Rev. Lett. 53 (1984) 644.
   J.B. Kogut, J. Polony, H.W. Wyld and D.K. Sinclair, Phys. Rev. Lett. 54 (1985) 1980.

4. A. Iwazaki, Phys. Lett. 159B (1985) 348.

5. Y. Morikawa and A. Iwazaki, LBL preprint LBL-20175 to be published in Phys. Lett. B.