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IN MICROCANONICAL SIMULATIONS

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Supercooled States and Order of Phase Transitions in Microcanonical Simulations

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Abstract

In microcanonical simulations, we propose an improved method to determine orders of phase transitions. We put friction terms in Hamilton's equations and continuously decrease the temperature of a system. Then, beyond a critical point of first order, this system is supercooled. We show that an appropriate choice of the friction coefficient leads to maximally enhanced S shaped curve of the internal energy vs. inverse temperature.

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Recently, microcanonical simulations have been used as a powerful method for numerical calculations in lattice gauge theories.[1] Notably, it provides a new method for the distinction of first order phase transitions from second (or higher) order phase transitions.[2),3] These distinctions have been also made in Monte Carlo simulations, for example, by examining the continuity of the internal energy at a critical point. However, the discontinuity in first order phase transitions may be smoothed out by finite volume effects. Hence, it is favorable to have a method of making a distinction, which works well even in a finite volume.

According to microcanonical simulations, we can find the internal energies of supercooled (or superheated) metastable states.[2),3] Namely, for a system with sufficiently small volume, its internal energy $\langle S \rangle$ ($\langle\ \rangle$ implies an average over a microcanonical ensemble[4]) becomes a multi-valued function of temperature β^{-1} beyond a critical point of a first order phase transition. 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 energies between the two phases prevent the decay of the metastable states in the system with a sufficiently small volume. The multi-valuedness of $\langle S \rangle$ is revealed by examining the, so-called, S-shaped curve[2),3] in the $\langle S \rangle$ vs. β plane. On the other hand, the multi-valuedness of $\langle S \rangle$ is not expected around a critical point of second order. The reason is that the internal energy is smooth at this critical point.

In this letter we shall propose an improved method of discovering the S-shaped behavior, in that the S shape is enhanced more than in the previous method (Heller et al.[2]). Furthermore, we can perform complete calculations

necessary for the distinction of the order of the phase transition much faster with our method than with the previous method. Our method is easy to understand intuitively.

Before explaining our method, first let us briefly sketch the microcanonical simulation. We consider a pure U(1) lattice gauge theory with the action $\beta S(U)$ in 4 dimensional space. (β^{-1} is a coupling constant, which we shall call temperature.) The generalization of our method to other lattice models is straightforward. The Hamiltonian used in the microcanonical simulation is

$$H_m = \sum_{a=1}^{N} \frac{p_a^2}{2} + S(U) \tag{1}$$

where p_a is a conjugate momentum with respect to a variable θ_a on a link a (a link variable U_a is defined as $U_a \equiv e^{i\theta_a}$). In eq.(1), N is the total number of links. In the simulation, we have to solve the following Hamilton's equations

$$\frac{dp_a}{d\tau} = -\frac{\partial H_m}{\partial \theta_a} \quad \text{and} \quad \frac{d\theta_a}{d\tau} = \frac{\partial H_m}{\partial p_a} \tag{2}$$

where τ is a fictitious time. A prominent feature of the microcanonical simulation is that the temperature β^{-1} is a measured quantity and not a given constant. The temperature can be measured, through the equipartition theorem, as

$$\frac{N_i}{2\beta} = \lim_{T\to\infty} \frac{1}{T} \int_0^T \left(\sum_{a=1}^{N} \frac{p_a^2}{2} \right) d\tau \tag{3}$$

where N_i is the number of independent degrees of freedom. If we take values $p_a = 0$ for all a as an initial condition in solving Hamilton's equations, N_i should be $n^4 \times (4-1)$; n^4 is the number of lattice sites.

The expectation value $\langle f(U) \rangle$ can be obtained in the same way as in eq.(3),

$$\langle f(U) \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T f(U(\tau)) d\tau \quad . \tag{4}$$

Now we shall explain our method, by which we can distinguish clearly the orders of the phase transitions. First, we thermalize the system above the critical point. Then, putting friction terms into Hamilton's equations (see eq.(5)), we continuously decrease the energy of the system. Evidently the decrease of the energy leads to the decrease of the temperature. That is, the system is cooled by the friction. When the temperature comes down below the critical point of first order, the system can be supercooled. Further decreasing the energy leads to a transition from the supercooled metastable state to a stable state. This transition is accompanied by the release of a latent heat. Since the latent heat increases the temperature of the system, we can obtain the S-shaped curve in the $\langle S \rangle$ vs. β plane.

To what extent it is supercooled depends on the rate at which the energy is decreased (the coefficient of friction terms in eq.(5)). If the energy is decreased too slowly, the system will not be supercooled sufficiently, and thus the supercooled state releases only a small amount of its latent heat in the subsequent transition. The resultant $\langle S \rangle$ vs. β curve will not have a distinct S shape. On the other hand, the energy may not be decreased too rapidly. This is because the latent heat released in the subsequent

transition will be absorbed in the friction energy without heating the system itself. Hence, we cannot also clearly identify the S-shaped behavior. Therefore, we must choose an appropriate rate with which the energy of the system is decreased. Such a choice may be easily accomplished. (We have performed the calculations with several different rates.)

Anyway, we can identify a first order phase transition by use of this method while, if the phase transition is of the second (or higher) order, we don't get any S-shaped behavior. The reason is that in this case there are no supercooled (or superheated) states around the critical point. Therefore, the identification of the order of the phase transition can be made clearly. As we shall show below, by using our method, we can amplify an S-shaped curve compared with one obtained previously.[2)]

In our actual procedure, the friction terms are put into Hamilton's equations as follows,

$$\frac{dp_a}{d\tau} = -\frac{\partial H_m}{\partial \theta_a} + C' p_a \quad \text{and} \quad \frac{d\theta_a}{d\tau} = \frac{\partial H_m}{\partial p_a} \tag{5}$$

$$\text{with} \quad C' \equiv C_0 / \sum_{a=1}^{N} p_a^2$$

where C_0 is a constant which determines the rate of decreasing the energy,

$$\frac{dH_m}{d\tau} = -C_0 \quad . \tag{6}$$

It is stressed that C_0 should be chosen such that $-H_m/(dH_m/d\tau)(=E/C_0)$ is much larger than the relaxation time of the system. (E is a typical energy of the system.) This is because the continuous decrease of the energy should proceed while preserving the equilibrium of the system.

We have examined our method by using U(1) lattice gauge theories with lattice size of 4^4. The action is

$$\beta S = \sum_P \beta \left(\left(1 - \frac{1}{2}(U_p + U_p^\dagger)\right) + \lambda \left(1 - \frac{1}{2}\left(U_p^2 + U_p^{\dagger 2}\right)\right)\right) ,$$

$$U_p \equiv \prod_{a \in p} e^{i\theta_a} \tag{7}$$

where P indicates a plaquette and λ is a parameter which has been taken as both $\lambda = 0$ and $\lambda = 1$ in our computations. In the case of $\lambda = 0$ the system undergoes a second order phase transition at $\beta \simeq 1$. On the other hand, in the case of $\lambda = 1$, the system undergoes a first order phase transition at $\beta \simeq 0.6$.[5] We have used the Leap-Frog method for solving Hamilton's equations in which a discrete time step $\Delta\tau$ has been taken as $\Delta\tau = 1/100$.

We have measured the temperature β^{-1} by taking an average of kinetic energy over an appropriately finite time interval T. At the same time, using the identical time interval T, we also have measured the internal energy $\langle S \rangle$. Hence, we have obtained $\langle S \rangle$ as a function of β. In Fig.1-a ~ Fig.1-c, we show the results of using various time intervals in case of $\lambda = 0$ and $C_0 = 10$. We can see thermal fluctuations, which imply that the time interval T = 100 is shorter than the relaxation time. These figures suggest that the relaxation time is about 1000 in units of $\Delta\tau = 1/100$. Since the energy of the system is about 1000 at $\beta \simeq 1$, the rate of decreasing energies $E/C_0 \simeq 100$ is longer than the relaxation time. (Note that T should be chosen as $E \gg C_0 \times T \times \Delta\tau$, because averages over unreasonably large T smooth out effects of various β.)

It is worthwhile to state that in our method the measurement of both <S> and ß can be performed continuously with the fictitious time. Therefore, we have obtained many data points as shown in the figures.

Next, we have measured <S> in both cases of $\lambda = 0$ and $\lambda = 1$, using $C_0 = 10$ and $T = 2000$. The results are shown in Fig.2 and Fig.3 (curve A). We find a clear distinction between these curves. That is, the curve representing the first order phase transition (Fig.3) has a typical S shape, while the curve representing the second order phase transition (Fig.2) doesn't have such a shape.

Let us compare our curve A with the curve B obtained with the previous method.[2] The S shape of the curve B is less clear than ours. This is due to the use of a slow rate of decrease of the energy in previous calculations. (The previous method is interpreted to correspond to our method with a rate of slowly decreasing energy.) Therefore, the system was supercooled less sufficiently than in our case, and it released only a small amount of the latent heat. It should be stressed that we have a peculiar interest in the existence of the supercooled state and not in the "equilibrium supercooled state," which may exist in the system with a sufficiently small volume as in our case. Hence, the discrepancy between our result and the previous one[2] around a critical pont does not imply a looseness of our method. Indeed, our curve A almost coincides with the curve B in the whole region of ß depicted in the figure except in the neighborhood of the critical point.

The curve C in Fig.3 represents the behavior of the system when we have chosen a slower rate of energy decrease ($C_0 = 5$). As expected, the system is less supercooled so that the subsequent transition releases a smaller amount of the latent heat. Consequently, the S shape becomes smaller than the one of curve A, and it approaches that of curve B even more.

It should be noticed that in both curves (A and C), we are able to identify clearly the existence of the supercooled state in the model ($\lambda = 1$). Furthermore, we stress that in the case of $C_0 = 10$ (curve A), it has taken 24000 time steps to perform the calculation of <S> in Fig.3. This number of time steps is, probably, of one order of magnitude less than time steps required in previous calculations.[3)]

To summarize, we have proposed an improved method for the distinction of orders of phase transitions. We have found that the method can enhance the S-shaped behavior of the first order phase transition. Furthermore, using the method, we can measure the internal energy, etc., in many points of β while reducing the time required to perform the calculation.

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Figure Captions

Fig.1-a ~ 1-c: $\langle S\rangle/N_p$ of U(1) gauge theory with the Wilson action. N_p is the number of the plaquette; $N_p = 6 \times 4^4$. $C_0 = 10$ (Fig.1-a ~ 1-c), T = 100 (Fig.1-a), T = 500 (Fig.1-b) and T = 1000 (Fig. 1-c).

Fig.2 : $\langle S\rangle/N_p$ of U(1) gauge theory with the Wilson action. $C_0 = 10$ and T = 2000.

Fig.3 : $\langle S\rangle/N_p$ of U(1) gauge theory with the mixed action. Curve A ($C_0 = 10$ and T = 2000), curve B quoted from ref.2 and curve C ($C_0 = 5$ and T = 4000).

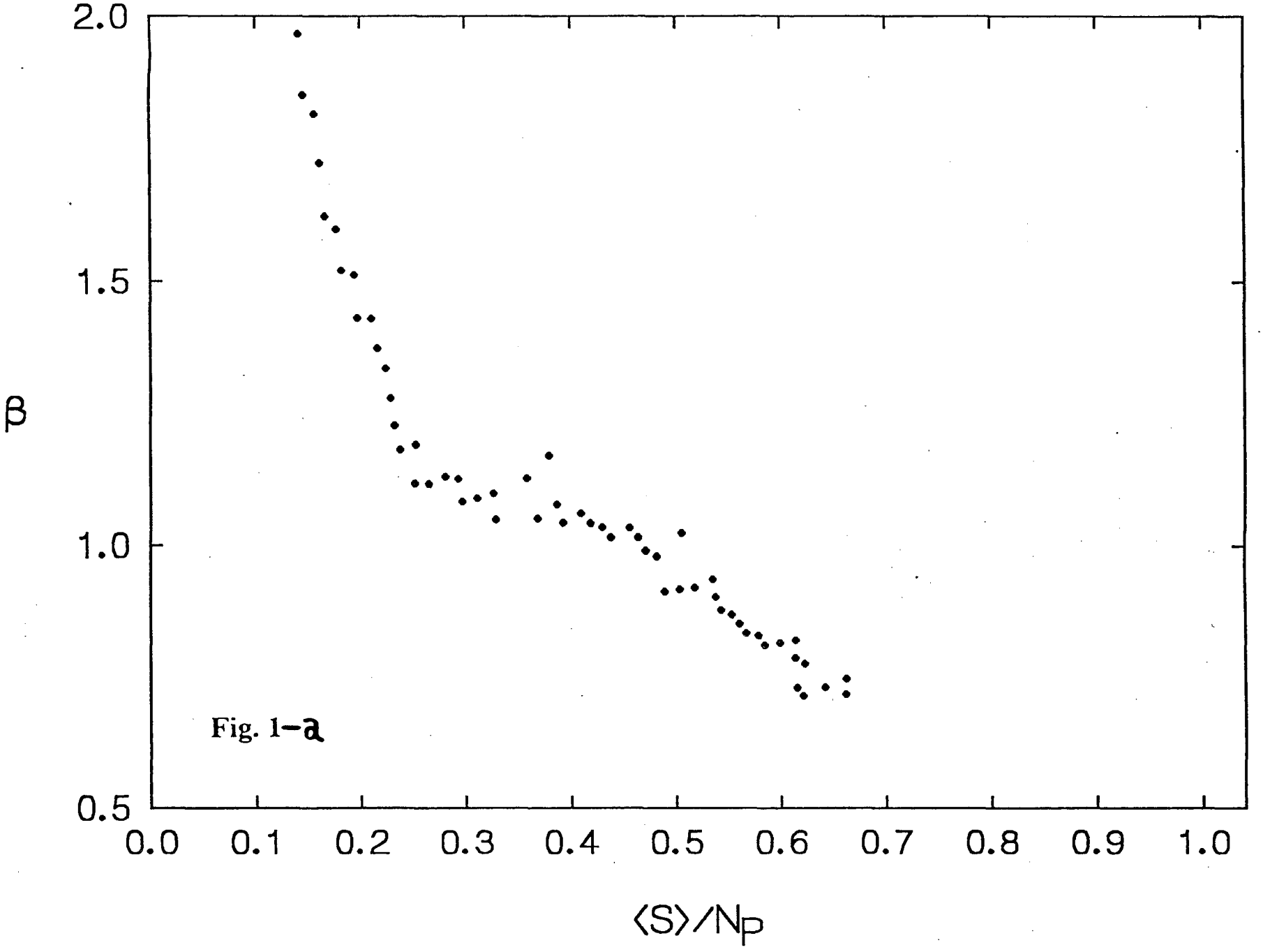

Fig. 1–a

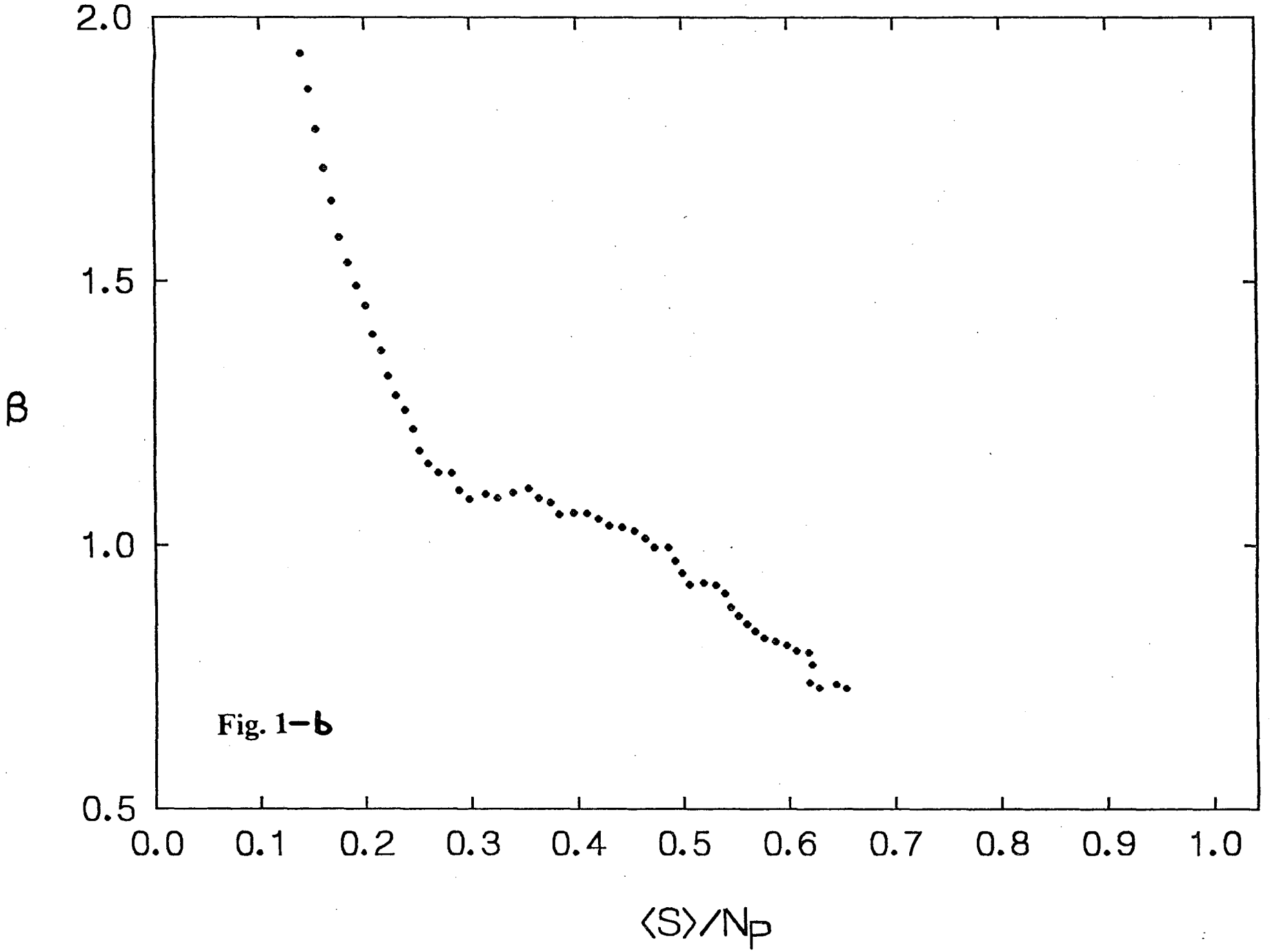

Fig. 1–b

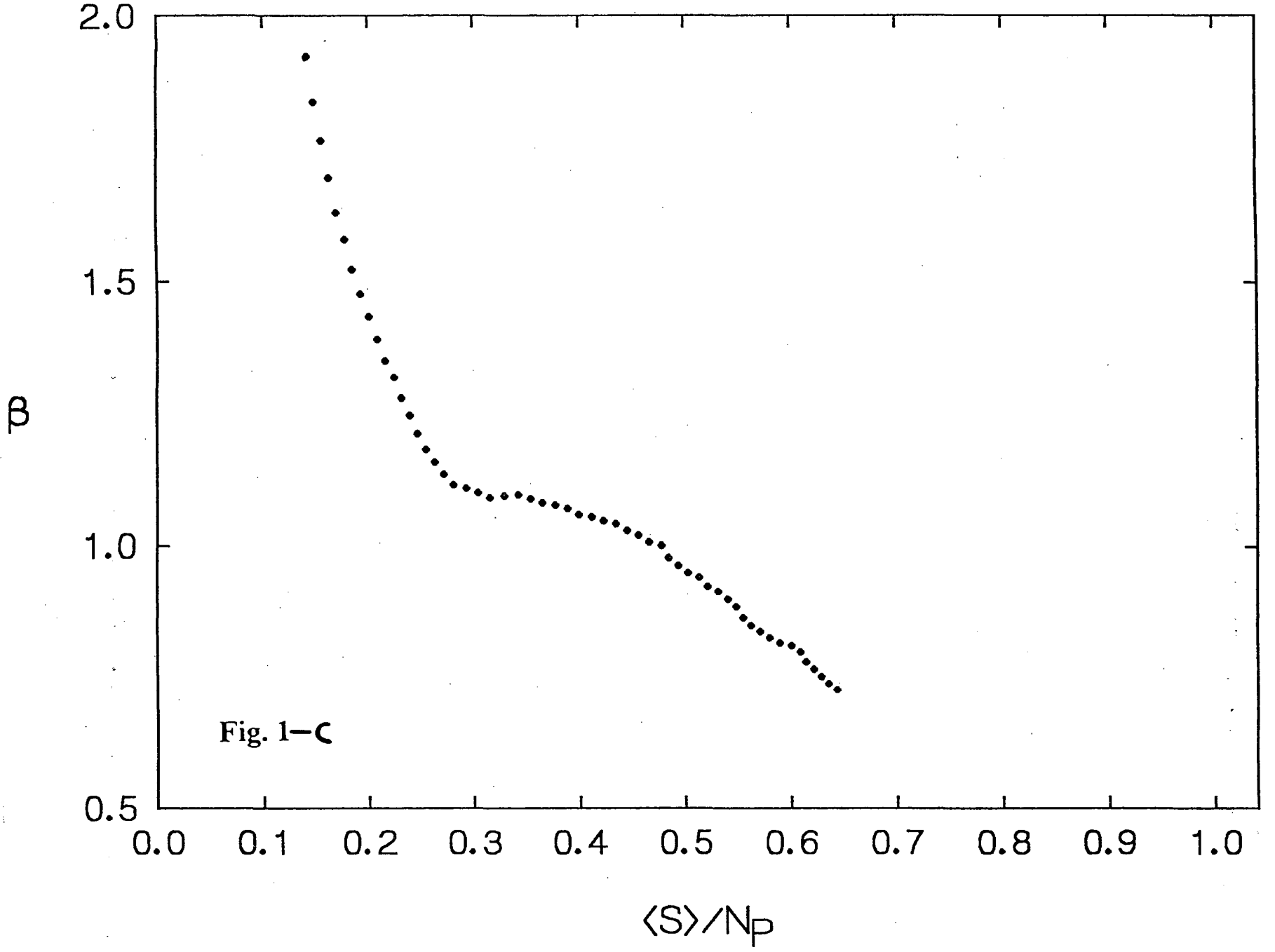

Fig. 1—c

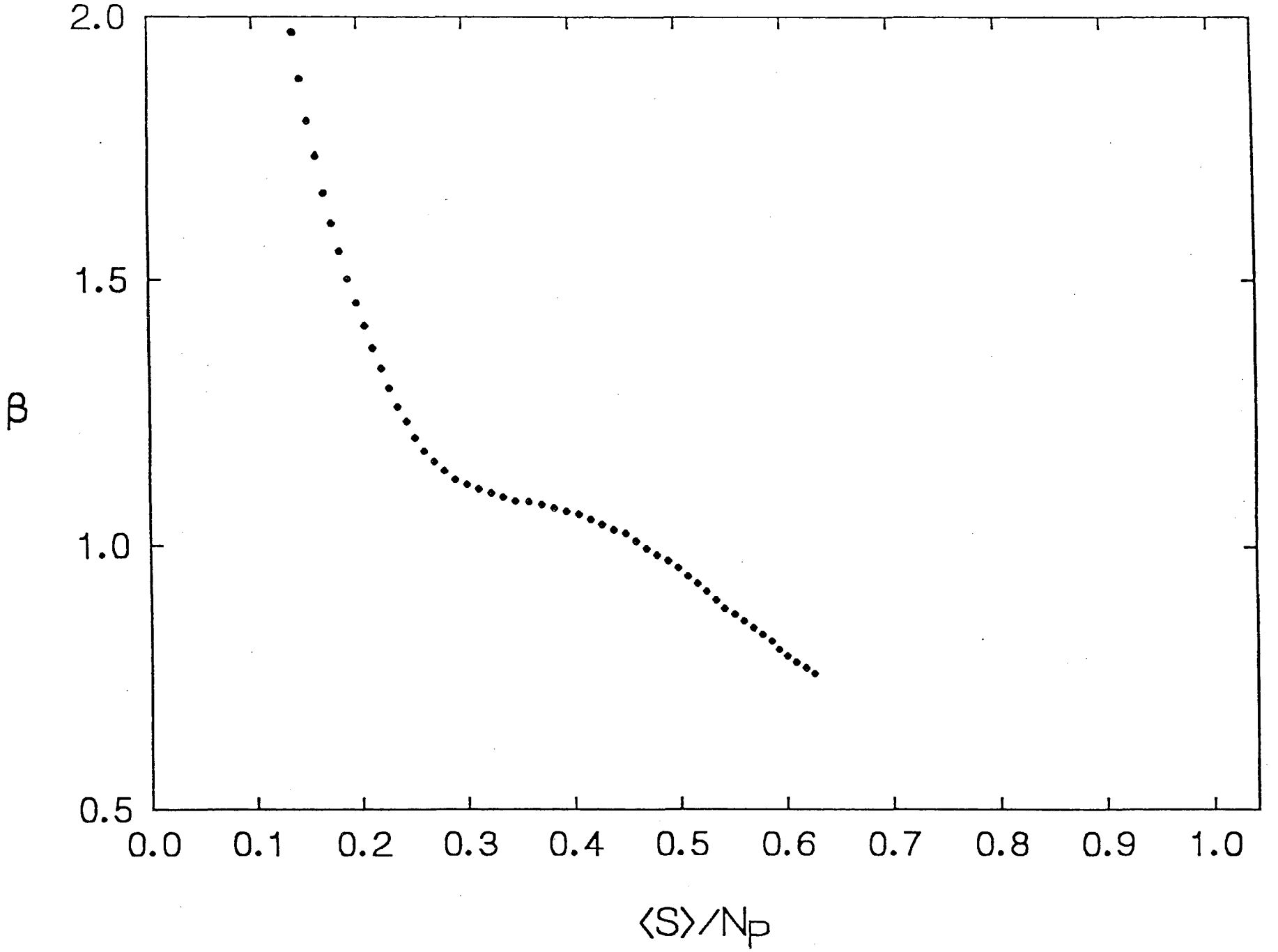

Fig. 2

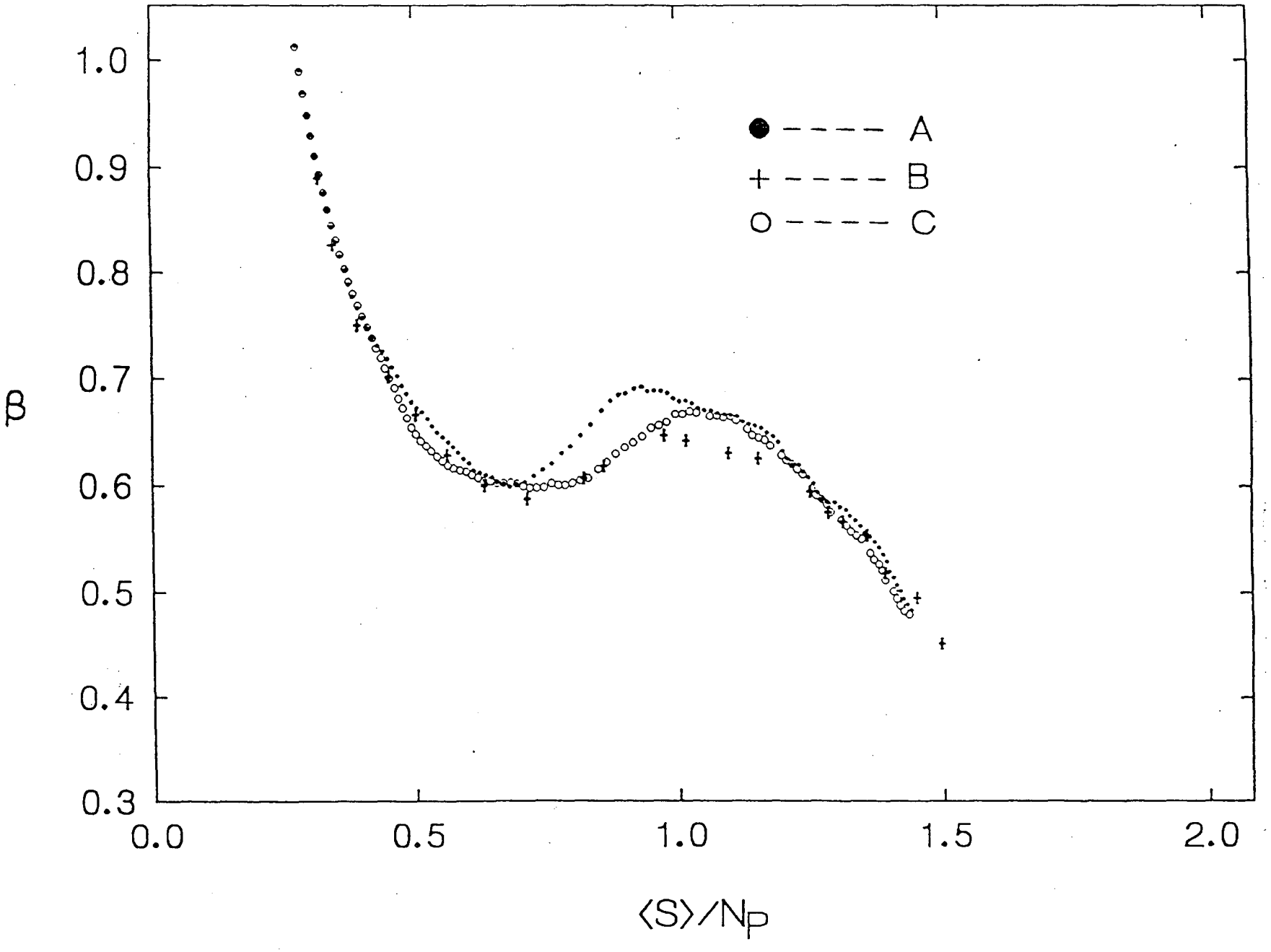

Fig. 3

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