Progress of Theoretical Physics, Vol. 43, No. 4, April 1970

On the Singularity of Dynamical Response and Critical Slowing Down

Masuo SUZUKI

Institute for Solid State Physics
University of Tokyo, Minato-ku, Tokyo

(Received August 18, 1969)

Phenomenological arguments on the critical slowing down is presented and "similarity law" is proposed on the indices of the critical slowing down. The similarity law is confirmed in linear spin chains near the critical field and in the kinetic Ising model near the critical temperature. It is exactly shown in the linear spin chains that the critical index of slowing down is different from that of the static susceptibility and that the dynamical susceptibility has a logarithmic singularity with respect to the frequency at the critical field and at zero temperature.

§ 1. Introduction

Although many investigations have been made on singularities of several kinds of dynamical phenomena near the critical point, there are very few that go essentially beyond a dynamical molecular field theory and afford a unified point of view on anomalies of dynamical responses in the vicinity of the critical point.

The purpose of this paper is to discuss the critical slowing down characteristic of dynamical critical phenomena from a unified point of view. In § 2, the main results of the Kubo linear response theory[1] are summarized for convenience to discuss the singularity of dynamical response and critical slowing down in the subsequent sections. In § 3, the formulation of relaxation time and its relation with dynamical susceptibility are given for the purpose of phenomenological arguments on the critical slowing down. "Similarity law" on the critical slowing down is proposed as a working assumption. In § 4, as an example, the dynamics of linear spin chains is investigated in detail near the critical field. The rigorous analysis yields that the critical index of slowing down is different from that of the corresponding susceptibility and that the "similarity law" holds with respect to the magnetization and partial energy. In § 5, we discuss the results obtained by our previous perturbational calculation[2] and those obtained by a computer simulation[3] from our point of view.

§ 2. The Kubo linear response theory

In the present paper, we discuss the singularity of dynamical response and critical slowing down, starting from the Kubo formula.[1] Thus, it is convenient to summarize the main results (relevant to our problems) or simple versions of the Kubo linear response theory.

The response $\Delta B(t)$ to an external periodic force $F(t)=F_0\cos(\omega t)$ conjugate to a physical quantity A is written as

$$\Delta B(t)=\mathrm{Re}\,\chi_{BA}(\omega)F_0e^{i\omega t}, \tag{2·1}$$

where the admittance $\chi_{BA}(\omega)$ is given by

$$\chi_{BA}(\omega)=\lim_{\varepsilon\to+0}\int_0^\infty\phi_{BA}(t)\,e^{-(i\omega+\varepsilon)}dt\,. \tag{2·2}$$

In the following, $\hbar$ will be replaced by 1; consequently, the response function $\phi_{BA}(\omega)$ is expressed as

$$\begin{aligned}\phi_{BA}(t)&=i\,\mathrm{Tr}[A,\rho]B(t)=-i\,\mathrm{Tr}\,\rho[A,B(t)]\\&=\int_0^\beta\mathrm{Tr}\,\rho\dot{A}(-i\lambda)B(t)\,dt\\&=-\int_0^\beta\mathrm{Tr}\,\rho A(-i\lambda)\dot{B}(t)\,d\lambda\,,\end{aligned} \tag{2·3}$$

where ρ is the canonical density matrix:

$$\begin{aligned}&\rho=\exp(-\beta(\mathcal{H}-\Psi)),\qquad\beta=1/k_BT\,,\\&\exp(-\beta\Psi)=\mathrm{Tr}\exp(-\beta\mathcal{H}),\end{aligned} \tag{2·4}$$

$\mathcal{H}$ is the Hamiltonian of the system, and $A(z)$ is the Heisenberg representation of A:

$$A(z)=e^{iz\mathcal{H}}Ae^{-iz\mathcal{H}}. \tag{2·5}$$

It is frequently convenient to use the relaxation function defined by

$$\Phi_{BA}(t)=\lim_{\varepsilon\to+0}\int_t^\infty\phi_{BA}(t')\,e^{-\varepsilon t'}dt' \tag{2·6a}$$

$$=i\int_t^\infty\langle[B(t'),A]\rangle dt' \tag{2·6b}$$

$$=-\int_t^\infty dt'\int_0^\beta d\lambda\langle A(i\lambda)\dot{B}(t')\rangle \tag{2·6c}$$

$$=\int_0^\beta d\lambda(\langle A(-i\lambda)B(t)\rangle-\lim_{t\to\infty}\langle A(-i\lambda)B(t)\rangle) \tag{2·6d}$$

$$=\int_0^\beta d\lambda\langle A(-i\lambda)B(t)\rangle-\beta\lim_{t\to\infty}\langle AB(t)\rangle \tag{2·6e}$$

$$=\int_0^\beta d\lambda\langle A(-i\lambda)B(t)\rangle-\beta\langle A^0B^0\rangle \tag{2·6f}$$

$$=\{1/\sum_i e^{-\beta E_i}\}\sum_{n,m}\langle n|A|m\rangle\langle m|B|n\rangle e^{-it(E_m-E_n)}\frac{e^{-\beta E_n}-e^{-\beta E_m}}{E_m-E_n}, \tag{2·6g}$$

where $|n\rangle$ is an eigenstate of the Hamiltonian with an eigenvalue E_n, A^0 and B^0 are the diagonal parts of A and B with respect to $\mathcal{H}$, and the average $\langle\cdots\rangle$ means the canonical average defined by

$$\langle A\rangle = \mathrm{Tr}\,\rho A\,. \tag{2·7}$$

In terms of the relaxation function, the response function $\chi_{BA}(\omega)$ can be written as

$$\chi_{BA}(\omega) = -\lim_{\varepsilon\to+0}\int_0^\infty \dot{\Phi}_{BA}(t)\,e^{-(i\omega+\varepsilon)t}dt \tag{2·8a}$$

$$=\Phi_{BA}(0) - i\omega\lim_{\varepsilon\to+0}\int_0^\infty \Phi_{BA}(t)\,e^{-(i\omega+\varepsilon)t}dt \tag{2·8b}$$

$$= -\lim_{\varepsilon\to+0}\int_0^\infty dt\int_0^\beta d\lambda e^{-(i\omega+\varepsilon)t}\frac{d}{dt}\langle AB(t+i\lambda)\rangle \tag{2·8c}$$

$$=i\lim_{\varepsilon\to+0}\int_0^\infty e^{-(i\omega+\varepsilon)t}(\langle AB(t+i\beta)\rangle - \langle AB(t)\rangle)\,dt \tag{2·8d}$$

$$=i\lim_{\varepsilon\to+0}\int_0^\infty e^{-(i\omega+\varepsilon)t}\langle[B(t),A]\rangle dt \tag{2·8e}$$

$$=\sum_{n,m}\frac{A_{mn}B_{nm}}{\omega+\omega_{mn}+i\varepsilon}(e^{-\beta E_n}-e^{-\beta E_m}), \tag{2·8f}$$

with $A_{mn}=\langle m|A|n\rangle/(\Sigma e^{-\beta E_i})^{1/2}$. In particular, the static response $\chi_{BA}(0)$ is given by

$$\chi_{BA}(0) = \Phi_{BA}(0) \tag{2·9a}$$

$$=\int_0^\beta d\lambda\{\langle AB(i\lambda)\rangle - \lim_{t\to\infty}\langle AB(t+i\lambda)\rangle\} \tag{2·9b}$$

$$=i\lim_{\varepsilon\to+0}\int_0^\infty e^{-\varepsilon t}(\langle AB(t+i\beta)\rangle - \langle AB(t)\rangle)\,dt \tag{2·9c}$$

$$=i\lim_{\varepsilon\to+0}\int_0^\infty e^{-\varepsilon t}\langle[B(t),A]\rangle dt\,, \tag{2·9d}$$

which should be compared with the isothermal response defined by

$$\chi_{BA}^T=\int_0^\beta d\lambda\{\langle AB(i\lambda)\rangle - \langle A\rangle\langle B\rangle\}. \tag{2·10}$$

The difference of the two response functions is expressed as

$$\chi_{BA}^T-\chi_{BA}(0) = \lim_{t\to\infty}\int_0^\beta d\lambda\langle AB(t+i\lambda)\rangle - \beta\langle A\rangle\langle B\rangle$$

$$=\beta\{\lim_{t\to\infty}\langle AB(t)\rangle - \langle A\rangle\langle B\rangle\} \tag{2·11}$$

in terms of Eqs. (2·9b) and (2·10). Thus, the two response functions are equal if the system is "ergodic" in the sense that

$$\lim_{t\to\infty} \langle AB(t)\rangle = \langle A\rangle\langle B\rangle\,. \tag{2·12}$$

Some rigorous examples will be shown to illustrate these situations in § 4.

§ 3. Phenomenological arguments on the critical slowing down

3. 1 *Relaxation Time*

In general, the critical slowing down of a physical quantity A is manifested by the anomalously long relaxation time τ_A of the quantity A. As the relaxation time τ_A is defined by the time integral of the corresponding relaxation function $\Phi_{AA}(t)$ with some weight, it is useful to study the properties of the relaxation function, particularly various kinds of its time integrals.

1. If A and B are both Hermitian, then

$$\Phi_{BA}(t) = \text{real} \qquad \text{and} \qquad \int_0^\infty \Phi_{AA}(t)\,dt \geq 0\,. \tag{3·1}$$

A simple proof for the first equation was given by Kubo.[1] It is also easily found from the following matrix-element representation:

$$\Phi_{BA}(t) = \sum_{m,n}\{R_{mn}\cos(\omega_{mn}t) - I_{mn}\sin(\omega_{mn}t)\} + i\sum_{m,n}\{R_{mn}\sin(\omega_{mn}t) + I_{mn}\cos(\omega_{mn}t)\}\,, \tag{3·2}$$

where

$$R_{mn} = \frac{1}{2}(A_{nm}B_{mn} + A_{mn}B_{nm})F_{mn}\,,$$

$$I_{mn} = \frac{1}{2i}(A_{nm}B_{mn} - A_{mn}B_{nm})F_{mn}\,, \tag{3·3}$$

$$A_{mn} = \langle m|A|n\rangle / \{\sum_i e^{-\beta E_i}\}^{1/2}$$

and

$$F_{mn} = (e^{-\beta E_n} - e^{-\beta E_m})/\omega_{mn}\,, \qquad \omega_{mn} = E_m - E_n\,, \tag{3·4}$$

which is easily derived from Eq. (2·6g). Obviously the imaginary part of Eq. (3·2) vanishes owing to the odd symmetry of the above matrix-element representation. Thus, the time integral of the relaxation function is given by

$$\int_0^\infty \Phi_{BA}(t)\,dt = \frac{\pi\beta}{2}\sum_{m,n}(A_{nm}B_{mn} + B_{nm}A_{mn})e^{-\beta E_n}\delta(\omega_{mn})\,. \tag{3·5}$$

In particular, for $A=B$, we obtain

$$\int_0^\infty \Phi_{AA}(t)\,dt = \pi\beta\sum |A_{nm}|^2 e^{-\beta E_n}\delta(\omega_{mn}) \geq 0\,. \tag{3·6}$$

That is, the time integral of the relaxation function $\Phi_{AA}(t)$ is usually positive and it vanishes only when all the secular parts of the quantity A are zero (i.e. $A_{nm}=0$ for $E_m=E_n$), as is the case of $A=\dot{B}=i[\mathcal{H}, B]$.

2. It is shown in the same way as in 1 that the time integral of the relaxation function with a weight function t is given by

$$\int_0^\infty \Phi_{BA}(t)\, tdt=\sum_{m,n} A_{nm}B_{mn}(e^{-\beta E_m}-e^{-\beta E_n})(\omega_{mn}+i\varepsilon)^{-3}. \tag{3·7}$$

In particular, for $A=B=$Hermitian, we find that the time integral is negative:

$$\int_0^\infty \Phi_{AA}(t)\, tdt=-\sum_{n,m}|A_{nm}|^2F_{nm}\omega_{mn}^{-2}<0\,. \tag{3·8}$$

On the other hand, the initial value of the relaxation function is positive:

$$\Phi_{AA}(0)=\sum_{n,m}|A_{nm}|^2F_{mn}>0 \tag{3·9}$$

for $A=$Hermitian. This means that the value of the relaxation function becomes negative in some ranges of the time variable t.

3. The above results can be easily extended to the following form:

$$\int_0^\infty \Phi_{BA}(t)\, t^{k-1}dt=i^k\sum_{n,m} A_{nm}B_{mn}(e^{-\beta E_n}-e^{-\beta E_m})(\omega_{mn}+i\varepsilon)^{-k-1}. \tag{3·10}$$

In particular, we find that

$$\int_0^\infty \Phi_{AA}(t)\, t^{2k}dt=(-1)^k\pi\beta(2k)!\sum_{n,m}|A_{nm}|^2e^{-\beta E_n}\omega_{mn}^{-2k}\delta(\omega_{mn}) \tag{3·11}$$

and

$$\int_0^\infty \Phi_{AA}(t)\, t^{2k-1}dt=(-1)^k(2k-1)!\sum_{n,m}|A_{nm}|^2F_{mn}\omega_{mn}^{-2k} \tag{3·12}$$

for an Hermitian operator A.

4. If A and B are both bounded, we find that

$$\int_0^\infty \Phi_{\dot{B}\dot{A}}(t)\, dt=i\langle[A, B]\rangle\,, \tag{3·13}$$

because the integral of the relaxation function in terms of Eq. (2·6b) is expressed as

$$\begin{aligned}\int_0^\infty \Phi_{\dot{B}\dot{A}}(t)\, dt&=i\int_0^\infty dt\int_t^\infty \langle[\dot{B}(t'), \dot{A}]\rangle dt'\\ &=-i\int_0^\infty \langle[B(t), \dot{A}]\rangle dt\\ &=i\langle[A, B]\rangle\,.\end{aligned} \tag{3·14}$$

Instead of the above derivation, we may use the matrix-element representation (2·6g); i.e.

$$\int_0^\infty \Phi_{\dot{B}\dot{A}}(t)\,dt = i\sum_{n,m} A_{nm}B_{mn}F_{nm}\omega_{mn} = i\langle[A, B]\rangle\,. \tag{3·15}$$

For $A=B$, we obtain

$$\int_0^\infty \Phi_{\dot{A}\dot{A}}(t)\,dt = 0\,. \tag{3·16}$$

This yields a theorem due to Kubo:[4)]

$$\int_0^\infty dt \int_0^\beta d\lambda \langle \dot{A}(-i\lambda)\,\dot{A}(t)\rangle = 0 \tag{3·17}$$

by noting the following property:

$$\lim_{t\to\infty} \langle \dot{A}\dot{B}(t)\rangle = 0\,, \tag{3·18}$$

if A and B are both bounded. This is proved as follows:

$$\begin{aligned}\lim_{t\to\infty} \langle \dot{A}\dot{B}(t)\rangle &= \lim_{T\to\infty}\frac{1}{T}\int_0^T \langle \dot{A}\dot{B}(t)\rangle dt \\ &= \lim_{T\to\infty}\frac{1}{T}\{\langle \dot{A}B(T)\rangle - \langle \dot{A}B\rangle\} \\ &= 0\,,\end{aligned} \tag{3·19}$$

or is proved from the expression

$$\langle \dot{A}\dot{B}(t)\rangle = \sum_{n,m} e^{-\beta E_n} A_{nm}B_{mn}\omega_{mn}^2 e^{it\omega_{mn}}. \tag{3·20}$$

5. The above results are extended in the following. If A and B are both bounded, then

$$\int_0^\infty \Phi_{\overset{(m)}{B}\overset{(n)}{A}}(t)\,t^{m+n-2}dt = (-1)^{m+1}(m+n-2)!\,i\langle[A, B]\rangle \tag{3·21}$$

and

$$\overset{(n)}{A} = \left[\frac{d^n}{dt^n}A(t)\right]_{t=0}$$

for $m+n\geq 2$, which are easily proved by mathematical induction or by substituting $\dot{B}$ instead of B in Eq. (3·23). In particular, when A and B commute, the above integral (3·21) vanishes.

6. It is also easily shown in the same way as in the above derivation that

$$\int_0^\infty \Phi_{\overset{(n)}{A}\overset{(n)}{A}}(t)\,dt = \int_0^\infty \Phi_{\overset{(n)}{A}\overset{(n)}{A}}(t)\,t^2dt = \cdots = \int_0^\infty \Phi_{\overset{(n)}{A}\overset{(n)}{A}}(t)\,t^{2n-2}dt = 0\,. \tag{3·22}$$

7. On the other hand, it should be noted that the following time integral does not vanish:

$$\int_0^\infty \Phi_{\substack{(m)(n)\\ B\ \ A}}(t)\,t^{m+n-1}dt = (-1)^m (m+n-1)!\,\Phi_{BA}(0). \tag{3·23}$$

Now, we are ready to define the relaxation time τ_A. For simplicity, hereafter, we treat only Hermitian operators. Then, the simplest definition of τ_A may be

$$\tau_A = \int_0^\infty \hat{\Phi}_{AA}(t)\,dt\,, \qquad \hat{\Phi}(t) = \Phi(t)/\Phi(0), \tag{3·24}$$

which is non-negative from the previous discussion given in 1. It should be noted that this might vanish completely as shown in Eq. (3·16). Thus, it is convenient to extend the definition of the relaxation time in the following:

$$\tau_A{}^{(n)} = \left\{\frac{\varepsilon_n}{(n-1)!}\int_0^\infty \hat{\Phi}_{AA}(t)\,t^{n-1}dt\right\}^{1/n}, \tag{3·25}$$

where

$$\varepsilon_n = \begin{cases} +1 & \text{for} \quad n=4k \quad \text{or} \quad 4k+1\,, \\ -1 & \text{for} \quad n=4k+2 \quad \text{or} \quad 4k+3\,. \end{cases} \tag{3·26}$$

Equations (3·11) and (3·12) yield

$$\tau_A{}^{(2k+1)} = \{\pi\beta \sum_{n,m} |A_{nm}|^2 e^{-\beta E_n}\omega_{mn}^{-2k}\delta(\omega_{mn})/\Phi_{AA}(0)\}^{1/(2k+1)} \tag{3·27}$$

and

$$\tau_A{}^{(2k)} = \{\sum_{n,m} |A_{nm}|^2 F_{mn}\omega_{mn}^{-2k}/\Phi_{AA}(0)\}^{1/(2k)}, \tag{3·28}$$

respectively.

As simple examples, Eqs. (3·22) and (3·23) lead to the results

$$\tau_{\dot{A}\dot{A}}^{(1)} = 0\,, \qquad \tau^{(1)}_{\substack{(n)(n)\\ A\ \ A}} = \tau^{(3)}_{\substack{(n)(n)\\ A\ \ A}} = \cdots = \tau^{(2n-1)}_{\substack{(n)(n)\\ A\ \ A}} = 0$$

and

$$\tau^{(2n)}_{\substack{(n)(n)\\ A\ \ A}} = \{\Phi_{AA}(0)/\Phi_{\substack{(n)(n)\\ A\ \ A}}(0)\}^{1/2n}, \tag{3·29}$$

if A is bounded.

From Eq. (3·8) or (3·28), the relaxation time $\tau_A{}^{(2)}$ *does not vanish*. Thus, it is sufficient for our purpose to make use of only $\tau_A{}^{(1)}$ or $\tau_A{}^{(2)}$. It is to be expected that if both relaxation times $\tau_A{}^{(1)}$ and $\tau_A{}^{(2)}$ are physically significant they show a common singularity near the critical point. An example in which we must use the definition of the relaxation time $\tau_A{}^{(2)}$ will be shown in the next section.

There is a simple relation between the relaxation time $\tau_A{}^{(n)}$ and the corresponding dynamical susceptibility $\chi_{AA}(\omega)$ as follows.

1. $$\tau_A{}^{(1)} = i\lim_{\omega\to 0}\{\chi_A(\omega)-\chi_A(0)\}/\{\omega\chi_A(0)\}, \tag{3·30}$$

because the susceptibility is expressed as

$$\chi_A(\omega) = \Phi_A(0) - i\omega \int_0^\infty \Phi_A(t)\, dt - i\omega \int_0^\infty \Phi_A(t)\,(e^{-i\omega t} - 1)\, dt \tag{3·31}$$

in terms of Eq. (2·8b).

2. When $\tau_A^{(1)} = 0$, we find the relation

$$\tau_A^{(2)} = [\lim_{\omega\to 0} \{\chi_A(\omega) - \chi_A(0)\} / \{\omega^2 \chi_A(0)\}]^{1/2}, \tag{3·32}$$

which will be used in § 4. Thus, the anomaly of the relaxation time is connected with the singularity of the frequency expansion in the susceptibility.

Finally, we remark that in stochastic models, the relaxation time $\tau_A (= \tau_A^{(1)})$ is formally written as

$$\tau_A = \left\langle A \frac{1}{L} A \right\rangle \Big/ \langle A^2 \rangle , \tag{3·33}$$

where L is an operator to describe the temporal development of the relevant system. The operator L is usually semi-positive definite as is illustrated in § 5, so that τ_A is always positive and does not vanish. Thus, the simplest definition of the relaxation time $\tau_A^{(1)}$ is sufficient in stochastic models.

3. 2 *Critical slowing down*

The relaxation time τ_A of the relevant quantity A in terms of Eqs. (2·6e) and (3·24), is given by

$$\tau_A = \int_0^\infty \hat{\Phi}_{AA}(t)\, dt , \qquad \hat{\Phi}(t) = \Phi(t) / \Phi(0) \tag{3·34}$$

and

$$\Phi_{AA}(t) = \beta\{(A, A(t)) - \lim_{t\to\infty} (A, A(t))\}, \tag{3·35}$$

where the canonical correlation (B, A) is defined by

$$(B, A) = \frac{1}{\beta} \int_0^\beta \langle e^{\lambda \mathcal{H}} B e^{-\lambda \mathcal{H}} A \rangle d\lambda . \tag{3·36}$$

In ergodic systems, the following relation holds:

$$\lim_{t\to\infty} (A, A(t)) = \langle A \rangle^2. \tag{3·37}$$

Thus, the relaxation function is expressed by the corresponding canonical correlation itself in ergodic systems: i.e.

$$\Phi_{AA}(t) = \beta(\delta A, \delta A(t)) \tag{3·38}$$

with $\delta A = A - \langle A \rangle$. Hereafter, we consider only ergodic systems and use the symbol A instead of δA, that is, $\langle A \rangle = 0$. The reduced relaxation function $\hat{\Phi}(t)$ can be written as

$$\hat{\Phi}_{AA}(t) \equiv \exp[\psi(t)] = (A, e^{it\mathcal{L}}A)/(A, A), \tag{3·39}$$

where $\mathcal{L}$ is the Liouville operator for the relevant system, and it is defined by

$$\mathcal{L}A = [\mathcal{H}, A] \equiv H^{\times}A . \tag{3·40}$$

The moment expansion of Eq. (3·39) yields

$$\hat{\Phi}_A(t) = \sum_{n=0}^{\infty} \frac{(it)^n}{n!} \cdot \frac{\mu_n}{\mu_0}, \qquad \mu_n = (A, \mathcal{L}^n A). \tag{3·41}$$

The use of the well-known cumulant expansion[5] gives the expression

$$\psi(t) = \sum_{n=1}^{\infty} \frac{(it)^n}{n!} \frac{\lambda_n(\xi)}{\mu_0{}^n}, \tag{3·42}$$

where

$$\begin{aligned} &\lambda_1(\xi) = \mu_1 , \\ &\lambda_2(\xi) = \mu_0\mu_2 - \mu_1{}^2, \\ &\lambda_3(\xi) = \mu_0{}^2\mu_3 - 3\mu_0\mu_1\mu_2 + 2\mu_1{}^3, \\ &\lambda_4(\xi) = \mu_0{}^3\mu_4 - 4\mu_0{}^2\mu_1\mu_3 - 3\mu_0{}^2\mu_2{}^2 + 12\mu_0\mu_1{}^2\mu_2 - 6\mu_1{}^4, \quad \text{etc.} \end{aligned} \tag{3·43}$$

and ξ indicates temperature T, a magnetic field H, or any other external parameter. Thus, the relaxation time τ_A is expressed as

$$\tau_A = \int_0^{\infty} \exp\left[\sum_{n=1}^{\infty} \frac{i^n \lambda_n(\xi)}{n!} \left(\frac{t}{\mu_0}\right)^n\right] dt = \mu_0 / R_A(\xi), \tag{3·44}$$

where

$$R_A{}^{-1}(\xi) = \int_0^{\infty} \exp\left[\sum_{n=1}^{\infty} \frac{i^n \lambda_n(\xi)}{n!} x^n\right] dx . \tag{3·45}$$

Under the conditions that

$$\textit{all } \lambda_n(\xi) = \textit{finite at the critical point } \xi_c , \tag{3·46}$$

and moreover that

$$R_A = R_A(\xi_c) = \text{finite (not zero)}, \tag{3·47}$$

the relaxation time shows the singularity

$$\tau_A \simeq \mu_0 / R_A = (A, A)/R_A = \chi_{AA}/(\beta R_A) \sim \varepsilon^{-\gamma_A} \tag{3·48}$$

with $\varepsilon = (\xi - \xi_c)/\xi_c$ near the critical point. That is, the index of the critical slowing down for the quantity A is equal to that of the corresponding susceptibility *in the above severe conditions.* It is easily found from Eqs. (3·43) that the condition (3·46) is equivalent to the relation

$$(A, \mathcal{L}^n A)(A, A)^{n-1} = \text{finite at } \xi_c \text{ for all } n , \tag{3·49}$$

which is satisfied in the dynamical molecular field theory.[6] Here the following decoupling method is valid:

$$\langle\!\langle \mathcal{L}^n \rangle\!\rangle \sim \langle\!\langle \mathcal{L} \rangle\!\rangle^n, \qquad \langle\!\langle Q \rangle\!\rangle = (A, QA)/(A, A). \tag{3·50}$$

The condition (3·49) is also satisfied in the situation where the quantity A happens to be a critical dynamical variable,[7] namely an asymptotic eigenvector of the Liouville operator $\mathcal{L}$ with an eigenvalue λ vanishing at ξ_c:

$$\mathcal{L}A \sim \lambda A, \qquad \lambda \sim (A, A)^{-1} \sim \chi_{AA}^{-1}. \tag{3·51}$$

A stochastic model with long-range interaction (where the molecular field approximation holds) is a nice example for the above situation.

However, the above conditions (3·49) and (3·40) are so much severe that it is unreasonable in general to expect that the relaxation time should be proportional to the static susceptibility in the vicinity of the critical point. That is, it should be remarked that in many cases the critical index of slowing down may be different from that of the static susceptibility. Such examples will be given in §§ 4 and 5.

Here, we note that all the odd moments in Eq. (3·41) do always vanish in the usual dynamical models described by the Liouville operator $\mathcal{L}$:

$$\mu_{2n+1} = (A, \mathcal{L}^{2n+1}A) = (-1)^n((\mathcal{L}^n A), \mathcal{L}(\mathcal{L}^n A)) = 0. \tag{3·52}$$

The second equality in the above equation is due to the property that the Liouville operator $\mathcal{L}$ is Hermitian in the sense that[8]

$$(A^*, \mathcal{L}B) = ((\mathcal{L}A)^*, B). \tag{3·53}$$

As the operator A and B are Hermitian ($A^* = A$) in our problem, the above equation can be written as

$$(A, \mathcal{L}B) = -(\mathcal{L}A, B). \tag{3·54}$$

The third equality in Eq. (3·52) is proved as follows. For a general operator A, we find that

$$\begin{aligned}
\beta(A, A\mathcal{H}) &= \int_0^\beta \langle e^{\lambda\mathcal{H}} A e^{-\lambda\mathcal{H}} A\mathcal{H} \rangle d\lambda \\
&= \int_0^\beta \langle e^{\lambda\mathcal{H}} \mathcal{H} A e^{-\lambda\mathcal{H}} A \rangle d\lambda \\
&= \int_0^\beta \langle e^{(\beta-\lambda)\mathcal{H}} \mathcal{H} A e^{-(\beta-\lambda)\mathcal{H}} A \rangle d\lambda \\
&= \int_0^\beta \langle e^{\beta\mathcal{H}} \mathcal{H} A e^{-\beta\mathcal{H}} e^{\lambda\mathcal{H}} A e^{-\lambda\mathcal{H}} \rangle d\lambda \\
&= \int_0^\beta \langle e^{\lambda\mathcal{H}} A e^{-\lambda\mathcal{H}} \mathcal{H} A \rangle d\lambda \\
&= \beta(A, \mathcal{H}A).
\end{aligned} \tag{3·55}$$

That is,

$$(A, \mathcal{L}A) = (A, \mathcal{H}A) - (A, A\mathcal{H}) = 0\,. \tag{3·56}$$

This is also derived from differentiating the following symmetry relation[9] and putting $t=0$,

$$(A, A(t)) = (A, A(-t))\,. \tag{3·57}$$

Thus, in dynamical systems, the expression $R_A(\xi)$ in Eq. (3·45) is seen to be real as arises necessarily from Eq. (3·1):

$$R_A^{-1}(\xi) = \int_0^\infty \exp\left[\sum_{n=1}^{\infty} \frac{(-1)^n}{(2n)!} \lambda_{2n}(\xi)\, x^{2n}\right] dx\,. \tag{3·58}$$

In stochastic models, a semi-positive definite operator L should be used instead of the operator $(-i\mathcal{L})$ in the above discussions. That is, the coefficient $R_A(\xi)$ in the expression (3·44) of the relaxation time is given by

$$R_A^{-1}(\xi) = \int_0^\infty \exp\left[\sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \lambda_n(\xi)\, x^n\right] dx\,. \tag{3·59}$$

In the stochastic kinetic Ising model, Abe[10] argued that a relaxation time associated with the initial decay is proportional to the susceptibility. Although the formal results are similar to each other, Abe's argument is quite different from ours in that the present relaxation time defined by Eq. (3·24) is associated with the long time behavior. Of course, they agree each other in the case when they show a single-exponential decay of a Lorentzian form essentially in the whole region of the time in stochastic models: $\hat{\Phi}(t) \sim \exp(-t/\tau)$.

In the kinetic Ising model,[2),6),10)~12)] all the moments remain finite[2),12)] and never vanish at ξ_c, and consequently the condition (3·46) does not hold. In fact, as is discussed in § 4, it is found from a perturbational calculation that the critical index of slowing down is different from that of the static susceptibility.

Finally, it should be remarked that the above argument is quite the same even if we use the other definitions of the relaxation time.

3. 3 *Similarity law on the critical slowing down*

In the previous subsection, we argued that the relaxation time should be proportional to the susceptibility in some severe conditions. Here, we discuss the general case on the critical slowing down in which the coefficient $R(\xi)$ is singular at ξ_c and consequently the critical index of slowing down may be different from that of the static susceptibility. Let us call the slowing down due to the static susceptibility χ_{AA} the "direct critical slowing down" or the "critical slowing down due to direct fluctuation", (which is called the thermodynamic critical slowing down in the case of temperature variable $(\xi = T)$), and call the remaining part the "indirect critical slowing down (or speeding up)" or the "kinetic slowing down (or speeding up)".

As will be confirmed in some examples given in the subsequent sections, the conjecture (or a working assumption) of the following similarity law is the motive of our investigation on the critical slowing down.

Similarity law: The indirect critical slowing down (or the kinetic slowing down) shows a common singularity near the critical point with respect to some physical variables in one "regular" system:

$$R_A(\xi) \sim (\xi - \xi_c)^{\phi_A}, \qquad \phi_A = \phi_B = \cdots = \phi \text{ (common)}. \tag{3·60}$$

This is easily expected from the consideration that the indirect critical slowing down is due to a kinetic effect characteristic of Liouville operator (or Hamiltonian) for the relevant system. In fact, the similarity law always holds in the results obtained by the simple theory discussed in the previous subsection in the sense that all $\phi_\alpha = \phi = 0$.

A system in which the above similarity law holds with respect to more than two variables may be called "regular" or "regular with respect to critical slowing down", and such variables satisfying the similarity law may be called "similar variables" or "variables similar with respect to critical slowing down".

The relevant problem is to investigate in what condition similar variables appear and consequently the system becomes regular. This is a very difficult problem. At present, we are to be satisfied with illustrating the similarity law in some examples.

§ 4. Example I—Linear spin chains

4.1 *Dynamical susceptibility*

In this section, a rigorous example is given to show the critical slowing down different from the singularity of the response function with respect to the magnetic field (i.e. near the critical field at $T=0$). It is also shown that the dynamical susceptibility $\chi(\omega)$ has a logarithmic divergence with respect to the frequency ω at the critical field H_c.

The Hamiltonian[13)~17)] we consider here is

$$\mathcal{H} = -\sum J_{jk} S_m{}^j S_{m+1}^k - \mu_B H \sum_{m=1}^{N} S_m{}^z, \tag{4·1}$$

where $S_m{}^j$ is the j-component of the spin operator at the m-th lattice site (the spin is equal to 1/2): J_{jk} is the symmetric tensor of the interaction constants associated with the transverse components ($j, k = x, y$), H the magnetic field and μ_B the Bohr magneton.

The Hamiltonian (4·1) is easily diagonalized by using the following transformation

$$S_n{}^- = S_n{}^x - iS_n{}^y = a_n{}^\dagger \prod_{m<n} (1 - 2a_m{}^\dagger a_m)$$

and

$$S_n^+ = S_n^x + iS_n^y = \prod_{m<n} (1-2a_m^\dagger a_m) a_n , \tag{4·2}$$

where $a_n^\dagger$ and a_n are respectively, the Fermi creation and annihilation operators. It is convenient to go over to the Fourier transforms of the Fermi operators a_n and $a_n^\dagger$:

$$a_n = \frac{1}{\sqrt{N}} \sum_k e^{ikn} a_k , \qquad a_n^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-ikn} a_k^\dagger . \tag{4·3}$$

Thus, the canonical u, v-transformation,

$$a_k = u_k c_k + v_k^* c_{-k}^\dagger , \qquad a_{-k} = -u_k c_{-k} + v_k^* c_k^\dagger ,$$
$$|u_k|^2 + |v_k|^2 = 1 , \tag{4·4}$$

yields the final diagonalization of the Hamiltonian as[14]

$$\mathcal{H} = \sum_k (c_k^\dagger c_k - \tfrac{1}{2}) \varepsilon_k , \tag{4·5}$$

where

$$\varepsilon_k = (A_k^2 + |B_k|^2)^{1/2},$$
$$A_k = \tfrac{1}{2}(J_{xx} + J_{yy}) \cos k - \mu_B H ,$$
$$B_k = i[\tfrac{1}{2}(J_{xx} - J_{yy}) + iJ_{xy}] \sin k , \tag{4·6}$$

and the coefficients u_k and v_k in Eq. (4·4) are given by

$$u_k = \frac{|B_k|}{[2\varepsilon_k(A_k+\varepsilon_k)]^{1/2}} , \qquad v_k = -\left[\frac{A_k+\varepsilon_k}{2\varepsilon_k}\right]^{1/2} \frac{|B_k|}{B_k} . \tag{4·7}$$

In general, the dynamical susceptibility $\chi(q, \omega)$ is given by the Kubo formula (2·8a):

$$\chi(q, \omega) = -\lim_{\varepsilon \to +0} \int_0^\infty \dot{\Phi}_q(t) e^{-(i\omega+\varepsilon)t} dt , \tag{4·8}$$

where the relaxation function $\Phi_q(t)$ is

$$\Phi_q(t) = \int_0^\beta d\lambda \langle M_q M_{-q}(t+i\lambda) \rangle - \beta \lim_{t\to\infty} \langle M_q M_{-q}(t) \rangle . \tag{4·9}$$

In the present model, noting that the magnetization M_q is expressed as

$$M_q = \mu_B \sum_n e^{iqn} S_n^z = \mu_B \left(\frac{N}{2} \delta(q) - \sum a_{k+q}^\dagger a_k \right) \tag{4·10}$$

and that

$$a_{k-q}^\dagger(z) a_k(z) = u_k u_{k-q}^* c_{k-q}^\dagger c_k \exp[iz(\varepsilon_{k-q} - \varepsilon_k)]$$
$$+ v_{k-q} v_k^* c_{-k+q} c_{-k}^\dagger \exp[iz(\varepsilon_{-k} - \varepsilon_{-k+q})]$$

$$+u_{k-q}^{*}v_{k}^{*}c_{k-q}^{\dagger}c_{-k}^{\dagger}\exp[iz(\varepsilon_{k-q}+\varepsilon_{-k})]$$
$$+u_{k}v_{k-q}c_{-k+q}c_{k}\exp[-iz(\varepsilon_{-k+q}+\varepsilon_{k})] \tag{4·11}$$

with $z=t+i\lambda$, we find easily that for $q\neq 0$,

$$\sum_{k,k'}\langle a_{k+q}^{\dagger}a_{k}a_{k'-q}^{\dagger}(z)a_{k'}(z)\rangle$$
$$=\sum_{k}\langle a_{k+q}^{\dagger}a_{k}(a_{k}^{\dagger}(z)a_{k+q}(z)+a_{-k-q}^{\dagger}(z)a_{-k}(z))\rangle$$
$$=\sum_{k}\{(1-n_{k})n_{k+q}\exp(iz(\varepsilon_{k}-\varepsilon_{k+q}))\times(|u_{k+q}|^{2}|u_{k}|^{2}-\phi(q,k))$$
$$+n_{k}(1-n_{k+q})\exp(-iz(\varepsilon_{k}-\varepsilon_{k+q}))\times(|v_{k+q}|^{2}|v_{k}|^{2}-\phi(q,k))$$
$$+n_{k}n_{k+q}\exp(-iz(\varepsilon_{k}+\varepsilon_{k+q}))\times(|u_{k+q}|^{2}|v_{k}|^{2}+\phi(q,k))$$
$$+(1-n_{k})(1-n_{k+q})\exp(iz(\varepsilon_{k}+\varepsilon_{k+q}))\times(|u_{k}|^{2}|v_{k+q}|^{2}+\phi(q,k))\}, \tag{4·12}$$

where

$$n_{k}=\langle c_{k}^{\dagger}c_{k}\rangle=1/(\exp(\beta\varepsilon_{k})+1),$$
$$\phi(q,k)=u_{k}u_{k+q}^{*}v_{k}^{*}v_{k+q}, \tag{4·13}$$

and we have used Wick's theorem at finite temperatures and the symmetry properties such as

$$\varepsilon_{-k}=\varepsilon_{k},\quad u_{-k}=u_{k},\quad v_{-k}=v_{k}\quad \text{and}\quad n_{-k}=n_{k}. \tag{4·14}$$

Therefore, we obtain the dynamical susceptibility in the form

$$\chi(q,\omega)=-\mu_{B}^{2}\lim_{\varepsilon\to+0}\int_{0}^{\infty}dt\int_{0}^{\beta}d\lambda e^{-(i\omega+\varepsilon)t}\frac{d}{dt}\sum_{k,k'}\langle a_{k+q}^{\dagger}a_{k}(a_{k'-q}^{\dagger}a_{k'})(t+i\lambda)\rangle$$
$$=\frac{1}{2}\mu_{B}^{2}\sum_{k}\Big[\{T(k+q)-T(k)\}\Big\{\frac{|u_{k+q}|^{2}|u_{k}|^{2}-\phi(k,q)}{\varepsilon_{k+q}-\varepsilon_{k}+\omega}+\frac{|v_{k+q}|^{2}|v_{k}|^{2}-\phi(k,q)}{\varepsilon_{k+q}-\varepsilon_{k}-\omega}\Big\}$$
$$+\{T(k+q)+T(k)\}\Big\{\frac{|u_{k+q}|^{2}|v_{k}|^{2}+\phi(k,q)}{\varepsilon_{k+q}+\varepsilon_{k}+\omega}+\frac{|u_{k}|^{2}|v_{k+q}|^{2}+\phi(k,q)}{\varepsilon_{k+q}+\varepsilon_{k}-\omega}\Big\}\Big] \tag{4·15}$$

with $T(k)=\tanh(\beta\varepsilon_{k}/2)$. In the case $J_{xx}=J_{yy}$ and $J_{xy}=0$, this agrees with the results obtained previously.[16] It is easily shown from direct calculation of $\chi(0,\omega)$ for $\omega\neq 0$ that

$$\lim_{q\to 0}\chi(q,\omega)=\chi(0,\omega)\equiv-\int_{0}^{\infty}\dot{\Phi}_{0}(t)e^{-i\omega t}dt, \tag{4·16}$$

where

$$\Phi_{0}(t)=2\mu_{B}^{2}\sum_{k}\frac{|u_{k}v_{k}|^{2}}{\varepsilon_{k}}T(k)\cos(2\varepsilon_{k}t). \tag{4·17}$$

In particular, the static susceptibility $\chi(q,0)$ is given by

$$\chi(q,0)=\frac{1}{2}\mu_B{}^2\sum_k\left\{\frac{T(k+q)-T(k)}{\varepsilon_{k+q}-\varepsilon_k}(|u_k|^2|u_{k+q}|^2+|v_k|^2|v_{k+q}|^2-2\phi(k,q))\right.$$
$$\left.+\frac{T(k+q)+T(k)}{\varepsilon_{k+q}+\varepsilon_k}(|u_{k+q}|^2|v_k|^2+|v_{k+q}|^2|u_k|^2+2\phi(k,q))\right\}. \qquad (4\cdot18)$$

Consequently, we find that

$$\lim_{q\to0}\chi(q,0)=\chi(0)+\chi', \qquad (4\cdot19)$$

where

$$\chi(0)=\frac{1}{2}\sum_k\frac{\partial^2\varepsilon_k}{\partial H^2}\tanh(\beta\varepsilon_k/2) \qquad (4\cdot20)$$

and

$$\chi'=\frac{\beta}{4}\sum_k\left(\frac{\partial\varepsilon_k}{\partial H}\right)^2\Big/\cosh^2(\beta\varepsilon_k/2). \qquad (4\cdot21)$$

That is,

$$\lim_{q\to0}\chi(q,0)=\chi^T, \qquad (4\cdot22)$$

where χ^T is the isothermal susceptibility calculated by Pikin et al.[14) This is a special case of the following relation

$$\chi(q,0)=\chi^T(q)\equiv\int_0^\beta d\lambda\{\langle M_qM_{-q}(i\lambda)\rangle-\langle M_q\rangle\langle M_{-q}\rangle\} \qquad (4\cdot23)$$

for $q\neq0$, which is easily shown from the ergodicity

$$\lim_{t\to\infty}\langle M_qM_{-q}(t)\rangle=\mu_B{}^2\lim_{t\to\infty}\sum_{k,k'}\langle a_{k+q}^\dagger a_k a_{k'-q}^\dagger(t)a_{k'}(t)\rangle$$
$$=0=\langle M_q\rangle\langle M_{-q}\rangle \qquad \text{for } q\neq0, \qquad (4\cdot24)$$

where we have used the theorem of Riemann and Lebesgue. In the case of $q=0$, we find easily that

$$\lim_{t\to\infty}(\langle MM(t)\rangle-\langle M\rangle^2)$$
$$=\mu_B{}^2\lim_{t\to\infty}\sum_k\{\langle a_k{}^\dagger a_k(a_k{}^\dagger(t)a_k(t)+a_{-k}^\dagger(t)a_{-k}(t))\rangle-2\langle a_k{}^\dagger a_k\rangle^2\}$$
$$=\mu_B{}^2\sum_k(|u_k|^2-|v_k|^2)^2n_k(1-n_k)$$
$$=\tfrac{1}{4}\sum_k(\partial\varepsilon_k/\partial H)^2/\cosh^2(\beta\varepsilon_k/2) \qquad (4\cdot25)$$

which yields the relation (4·22). From Eqs. (4·19), (4·21) and (4·22), the following inequality between the isothermal susceptibility and the isolated susceptibility holds:

$$\chi^T\geq\chi(0), \qquad (4\cdot26)$$

which has been proved in general by Falk[18] and Wilcox.[19] Thus, the ergodicity holds in our system only when $T\to 0$, in the sense that

$$\lim_{t\to\infty}\langle MM(t)\rangle=\langle M\rangle^2, \tag{4·27}$$

and *for $T>0$ the ergodicity does not hold in the present system, though the total magnetization is not a constant of motion.* This is because such a part of the Hamiltonian as does not commute with the total magnetization is of a special form; i.e. it connects only the two modes $a_k^\dagger$ and $a_{-k}^\dagger$.

4.2 *Singularity of dynamical susceptibility*

The real part of the dynamical susceptibility for $q=0$ is given by

$$\mathrm{Re}\,\chi(\omega)=\frac{2\mu_B^2}{\pi}P\int_0^\pi d\varphi\frac{|B(\varphi)|^2T(\varphi)}{\varepsilon(\varphi)\,(4\varepsilon^2(\varphi)-\omega^2)}, \tag{4·28}$$

where

$$\varepsilon(\varphi)=(A^2(\varphi)+|B(\varphi)|^2)^{1/2},\qquad T(\varphi)=\tanh\left(\frac{\beta}{2}\varepsilon(\varphi)\right),$$

$$A(\varphi)=\tfrac{1}{2}(J_{xx}+J_{yy})\cos\varphi-\mu_BH$$

and

$$|B(\varphi)|^2=[(J_{xx}-J_{yy})^2/4+J_{xy}^2]\sin^2\varphi\equiv J^2\gamma^2\sin^2\varphi\,. \tag{4·29}$$

The imaginary part of the susceptibility is

$$\mathrm{Im}\,\chi(\omega)=\frac{(\mu_BJ\gamma)^2}{\pi\omega}\int_0^\pi d\varphi\frac{\sin^2\varphi}{\varepsilon(\varphi)}T(\varphi)\left\{\delta(2\varepsilon(\varphi)-\omega)+\delta(2\varepsilon(\varphi)+\omega)\right\}. \tag{4·30}$$

The above susceptibility is easily found to satisfy the symmetry relations

$$\mathrm{Re}\,\chi(\omega,H)=\mathrm{Re}\,\chi(-\omega,H)=\mathrm{Re}\,\chi(\omega,-H)$$

and

$$\mathrm{Im}\,\chi(\omega,H)=-\mathrm{Im}\,\chi(-\omega,H)=\mathrm{Im}\,\chi(\omega,-H), \tag{4·31}$$

which are generally proved by Kubo.[1] The case of high temperature limit in the above expressions has been investigated in detail by Niemeijer.[15] Here, we are interested in the low temperature limit and the neighborhood of the critical field. In particular, we investigate the singularity of the real part of the dynamical susceptibility, in order to clarify the character of the critical slowing down.

It is easily shown that the real part of the dynamical susceptibility has the singularity in the form

$$\mathrm{Re}\,\chi(\omega,h,T=0)\simeq\frac{\mu_B^2}{2\pi J\gamma}f(\omega/2J\gamma,h) \tag{4·32}$$

for small ω and h, where

$$f(\omega, h)=P\int_h^a \frac{k^2}{\sqrt{h^2+k^2}}\frac{dk}{h^2+k^2-\omega^2}$$

$$=\begin{cases} \dfrac{\sqrt{D}}{2|\omega|}\log\left|\dfrac{|\omega|C-\sqrt{D}}{|\omega|C+\sqrt{D}}\right|+\dfrac{1}{2}\log\left|\dfrac{C+1}{C-1}\right| & \text{for } \omega^2\geq h^2, \\ -\dfrac{\sqrt{-D}}{|\omega|}\tan^{-1}\left(\dfrac{|\omega|C}{\sqrt{-D}}\right)+\dfrac{1}{2}\log\left|\dfrac{C+1}{C-1}\right| & \text{for } \omega^2<h^2, \end{cases} \tag{4·33}$$

where a is some constant of the order of unity, $C=(1-a^{-2}h^2)^{1/2}$, $D=\omega^2-h^2$, $h=\mu_B(H-H_c)/J\gamma$ and $\mu_B H_c=\frac{1}{2}(J_{xx}+J_{yy})$. For small ω and h, we obtain

$$f(\omega, h)\simeq\begin{cases} -\dfrac{\sqrt{\omega^2-h^2}}{|\omega|}\log(|\omega|+\sqrt{\omega^2-h^2})+\dfrac{\sqrt{\omega^2-h^2}-|\omega|}{|\omega|}\log|h| & \text{for } |\omega|\geq|h|, \\ -\log|h|-\dfrac{\sqrt{h^2-\omega^2}}{|\omega|}\tan^{-1}\dfrac{|\omega|}{\sqrt{h^2-\omega^2}} & \text{for } |\omega|<|h|. \end{cases} \tag{4·34}$$

In particular, the real part of the dynamical susceptibility shows the logarithmic singularity

$$\mathrm{Re}\,\chi(\omega, H_c, T=0)\sim-\log|\omega| \tag{4·35}$$

at the critical field H_c in the case of $\gamma\neq0$. The static susceptibility $\chi(0)$ has a logarithmic singularity with respect to the reduced field h:

$$\chi(0)\sim-\log|h| \qquad \text{for } \gamma\neq0 \text{ and for } T=0. \tag{4·36}$$

As the difference R of the isothermal susceptibility from the isolated susceptibility is finite at the critical field H_c, the isothermal susceptibility has the same singularity:

$$\chi^T\sim-\log|h|, \quad T=0 \tag{4·37}$$

for $\gamma\neq0$, as was pointed out by Pikin et al.[14] It is also easily shown from Eq. (4·18) that the wave-number dependent static susceptibility shows a logarithmic singularity

$$\chi(q, \omega=0, H=H_c, T=0)\sim-\log q \tag{4·38}$$

at the critical field and at $T=0$ for $\gamma\neq0$.

4.3 *On the critical slowing down*

In the present model, the system is "ergodic" with respect to the magnetization at the absolute zero temperature in the sense that

$$\lim_{t\to\infty}(M, M(t))=\langle M\rangle^2. \tag{4·39}$$

Thus, the relaxation time of the magnetization is defined by

$$\tau_M^2=-\int_0^\infty\{(\delta M, \delta M(t)/(M, M)\}tdt$$

$$=\lim_{\omega\to 0}\{\chi(\omega)-\chi(0)\}/\{\omega^2\chi(0)\}, \tag{4·40}$$

which reduces to

$$\tau_M{}^2=\left(\sum_k \frac{|B_k|^2}{4\varepsilon_k{}^5}\right)\bigg/\left(\sum_k \frac{|B_k|^2}{\varepsilon_k{}^3}\right)\sim h^{-2\Delta_M}, \qquad \Delta_M=1\,, \tag{4·41}$$

near the critical field at $T=0$, where the logarithmic singularity has been neglected at the above final expression. On the other hand, the exponent γ_M of the singularity of the fluctuation (M, M) is equal to zero ($\gamma_M=0$); $\chi(0)\sim h^{-\gamma_M}\sim -\log|h|$. Thus, the index of the kinetic critical slowing down becomes

$$\phi_M=\Delta_M-\gamma_M=1\,. \tag{4·42}$$

It should be noted that for the first time we have found a rigorous example in which the index of the critical slowing down Δ_M is different from that of the susceptibility ($\Delta_M>\gamma_M$). The existence of such an example is favorable to the previous results on the critical slowing down in the kinetic Ising model.[2)]

4.4 *Relaxation of partial energy*

In order to study whether the similarity law on the critical slowing down holds in the present system or not, we investigate the relaxation of a partial energy defined by

$$E=4\sum_i S_i{}^x S_{i+1}^x\,, \tag{4·43}$$

which is written as

$$E=\sum_n (a_n{}^\dagger a_{n+1}+a_{n+1}^\dagger a_n+a_n{}^\dagger a_{n+1}^\dagger+a_{n+1}a_n) \tag{4·44}$$

in terms of Eq. (4·2). The Fourier transform of the above equation (4·44) yields

$$E=\sum_k\{2\cos k a_k{}^\dagger a_k+i(a_k{}^\dagger a_{-k}^\dagger+a_{-k}a_k)\sin k\}. \tag{4·45}$$

With the use of u, v-transformation (4·4), we find that

$$E(t)=\sum_k (A_k' c_k{}^\dagger c_k+B_k' c_{-k}c_{-k}^\dagger+F_k{}^* e^{2i\varepsilon_k t}c_k{}^\dagger c_{-k}^\dagger+F_k e^{-2i\varepsilon_k t}c_{-k}c_k), \tag{4·46}$$

where

$$A_k'=2u_k{}^2\cos k+i(u_k{}^*v_k-u_kv_k{}^*)\sin k\,,$$

$$B_k'=2u_k{}^2\cos k-i(u_k{}^*v_k-u_kv_k{}^*)\sin k$$

and

$$F_k=2u_kv_k\cos k+i(u_k{}^2+v_k{}^2)\sin k\,. \tag{4·47}$$

The response function of the partial energy is given by

$$\chi_{EE}(\omega)=-\lim_{\varepsilon\to+0}\int_0^\infty dt\int_0^\beta d\lambda e^{-(i\omega+\varepsilon)t}\frac{d}{dt}\langle EE(t+i\lambda)\rangle$$

$$=4\lim_{\varepsilon\to+0}\int_0^\infty e^{-(i\omega+\varepsilon)t}dt\sum_k|F_k|^2\tanh\left(\frac{\beta}{2}\varepsilon_k\right)\sin(2\varepsilon_k t)$$

$$=\frac{8}{\pi}\int_0^\pi\frac{\varepsilon_k}{4\varepsilon_k{}^2-\omega^2}|F_k|^2\tanh\left(\frac{\beta}{2}\varepsilon_k\right)dk\,. \tag{4·48}$$

For simplicity, considering the case $J_{xy}=0$, we obtain

$$\chi_{EE}(\omega)=\frac{8J^2}{\pi}\int_0^\pi\frac{\sin^2 k}{\varepsilon_k(4\varepsilon_k{}^2-\omega^2)}\{(1-\gamma)\cos k-H/H_c\}^2dk \tag{4·49}$$

at $T=0$. In the same way as in the previous subsections, we find that

$$\chi_{EE}(0)\sim-\log|h|\,,\qquad \gamma_E=0 \tag{4·50}$$

and

$$\tau_E{}^2=\lim_{\omega\to0}\{\chi_{EE}(\omega)-\chi_{EE}(0)\}/\{\omega^2\chi_{EE}(0)\}\sim h^{-2\Delta_E},\qquad \Delta_E=1\,. \tag{4·51}$$

That is, the indices of the critical slowing down are equal to those of the magnetization:

$$\gamma_E=0\,,\qquad \Delta_E=1\qquad\text{and}\qquad \phi_E=1=\phi_M \tag{4·52}$$

for $\gamma\neq0$. Thus, the similarity law holds at least with respect to the variables M and E: i.e. they are "variables similar with respect to the critical slowing down" in this system.

§ 5. Example II—Kinetic Ising model

As an example of the critical slowing down with respect to temperature variable, a stochastic kinetic Ising model is discussed. We argue the difference between the singularity of the relaxation time for the magnetization of the system and that of the static susceptibility, on the basis of our previous perturbational calculation[2)] of the dynamical susceptibility, and also discuss the similarity law with respect to variables such as the magnetization, energy and energy-spin correlation with the use of the results obtained by a computer simulation.[3)]

(i) As is well known, in this model each spin is assumed to flip spontaneously with a transition probability which depends on the temperature and the configuration of surrounding spins, but the functional form of the transition probability is assumed to be the simplest. The master equation is given by

$$\frac{d}{dt}P(S_1,\cdots S_N;t)=\Gamma P(S_1,\cdots S_N;t)\,,\qquad S_i=\pm1\,, \tag{5·1}$$

where $P(S_1,\cdots S_N;t)$ is the transition probability to find the spins in the configuration $(S_1,\cdots S_N)$, and the operator Γ is defined by

$$\Gamma P(S)=-\sum_j W_j(S_j)P(S)+\sum_j W_j(-S_j)P(\cdots,-S_j,\cdots)\,. \tag{5·2}$$

The transition probability $W_j(S_j)$ is assumed to be[2),6)]

$$W_j(S_j)=\frac{1}{2\tau}(1-S_j\tanh\beta_B\sum_k J_{jk}S_k),\qquad \beta_B=1/k_BT. \tag{5·3}$$

It is convenient to use the following operator L:

$$L=\sum_k W_k(S_k)(1-P_k), \tag{5·4}$$

where P_k is an operator to flip the spin k, namely

$$P_kf(S_1,\cdots,S_k,\cdots)=f(S_1,\cdots,-S_k,\cdots). \tag{5·5}$$

The following relation between the operators Γ and L is easily derived:

$$\Gamma[f(S)P_0(S)]=-P_0(S)Lf(S),\qquad \Gamma P_0=0. \tag{5·6}$$

(ii) The critical slowing down of the relevant quantity η_q with wave number q is manifested by the following formula:

$$\tau_q=\int_0^\infty\frac{\langle\eta_q(t)\eta_q{}^*\rangle}{\langle\eta_q\eta_q{}^*\rangle}dt=\int_0^\infty\frac{\langle\eta_q{}^*e^{-Lt}\eta_q\rangle}{\langle\eta_q{}^*\eta_q\rangle}dt=\left\langle\eta_q{}^*\frac{1}{L}\eta_q\right\rangle\Big/\langle\eta_q{}^*\eta_q\rangle. \tag{5·7}$$

ii-1) Magnetization: the relaxation time for the magnitization $M=\mu_B\sum_j S_j$ is given by

$$\tau_M=\left\langle M\frac{1}{L}M\right\rangle\Big/\langle M^2\rangle\sim\varepsilon^{-\Delta M},\qquad \varepsilon=(T-T_c)/T_c. \tag{5·8}$$

If the index of the kinetic slowing down is expressed by ϕ_M, then we may put

$$\Delta_M=\gamma+\phi_M. \tag{5·9}$$

ii-2) Energy correlation: the relaxation time for the energy $\delta E=E-\langle E\rangle$ is given by

$$\tau_E=\left\langle\delta E\frac{1}{L}\delta E\right\rangle\Big/\langle(\delta E)^2\rangle\sim\varepsilon^{-\Delta E} \tag{5·10}$$

and

$$\Delta_E=\alpha+\phi_E, \tag{5·11}$$

where ϕ_E indicates the index of the kinetic slowing down for the energy.

ii-3) Energy-spin correlation below the Curie point T_c: the relaxation time for the energy-spin correlation is given by

$$\tau_{ME}=\left\langle\delta E\frac{1}{L}M\right\rangle\Big/\langle M\delta E\rangle\sim|\varepsilon|^{-\Delta ME}, \tag{5·12}$$

where

$$\Delta_{ME}=1-\beta+\phi_{ME} \tag{5·13}$$

and

$$\langle M\delta E\rangle \propto |\varepsilon|^{\beta-1}. \tag{5·14}$$

It is easy to derive the inequality

$$2\varDelta_{ME}-(\varDelta_M+\varDelta_E)\leq\alpha+2\beta+\gamma-2 \tag{5·15}$$

with the use of the following identity valid for a real parameter λ:

$$\left\langle(\lambda M+\delta E)\frac{1}{L}(\lambda M+\delta E)\right\rangle\geq 0\,. \tag{5·16}$$

(L: semi-positive definite)

If we accept the similarity assertion $\phi_M=\phi_E=\phi_{ME}=\phi$ in Eqs. (5·9), (5·11) and (5·13), we find the inequality[20]

$$\alpha+2\beta+\gamma\geq 2\,. \tag{5·17}$$

Conversely, if we make use of the equality $\alpha+2\beta+\gamma=2$, which is derived by the scaling law,[21] we obtain

$$\varDelta_M+\varDelta_E\geq 2\varDelta_{ME}\,. \tag{5·18}$$

(iii) In order to examine the nature of the kinetic slowing down, we studied high temperature expansions[2]

$$L=L_0-L', \qquad L_0=\frac{1}{2\tau}\sum_k(1-P_k),$$

$$L'=\frac{1}{2\tau}\sum_k S_k\tanh\left(\frac{1}{k_BT}\sum_j J_{kj}S_j\right)(1-P_k) \tag{5·19}$$

and

$$\left\langle M\frac{1}{L}M\right\rangle=\left\langle M\frac{1}{L_0-L'}M\right\rangle=\left\langle M\frac{1}{L_0}M\right\rangle+\left\langle M\frac{1}{L_0}L'\frac{1}{L_0}M\right\rangle+\cdots. \tag{5·20}$$

By applying the ratio method to the results obtained by high temperature expansions up to the ninth order in the two-dimensional Ising model, we have found that[2]

$$\varDelta_M=2.00\pm 0.05\,. \tag{5·21}$$

Therefore, the index of the kinetic slowing down, ϕ_M, is given by

$$\phi_M=\tfrac{1}{4}\,, \tag{5·22}$$

where we have used the value of the index $\gamma=7/4$ in the two-dimensional system.[22] Incidentally, we note that in the two-dimensional system the value of the index ϕ_M is the same as that of the index η (or $\eta\nu$) defined in the asymptotic equation

$$\langle S_0S_R\rangle\sim\frac{e^{-\kappa R}}{R^{2-d+\eta}}, \qquad \kappa=\xi_{\rm coher}^{-1}\sim\varepsilon^{\nu}. \tag{5·23}$$

Now, if we assume that the similarity law

$$\phi_M = \phi_E = \phi_{ME} = \phi \tag{5·24}$$

is valid in the present system, the following relations should hold:

$$\Delta_{ME} = 1 - \beta + \phi = \tfrac{9}{8}$$

and (5·25)

$$\Delta_E = \alpha + \phi = \tfrac{1}{4}\,.$$

(it contains a logarithmic divergence; namely $\tau_E \sim -\varepsilon^{1/4}\log\varepsilon$)

There are two ways to verify this assertion. One is to execute high temperature expansions for the energy correlation and energy-spin correlation in the same way as is shown in Eq. (5·20). The other is to make use of the results obtained by a computer simulation.[3] Figure 1 shows the relaxation time τ_M in the two-dimensional systems. The straight line in Fig. 1 gives an approximate value $\Delta_M \simeq 2$. As was pointed out by Ogita et al. far from the Curie point, however, the relaxation time becomes to be proportional to the susceptibility. This may imply that the kinetic slowing down becomes more and more conspicuous as the temperature approaches the critical point. On the other hand, the relaxation time of the energy, τ_E, is shown in Fig. 2, which seems to yield the conjectured value

$$\Delta_E = \tfrac{1}{4} \tag{5·26}$$

from the data close to the critical point. The results obtained by the computer simulation does not seem to be so accurate. At present, we

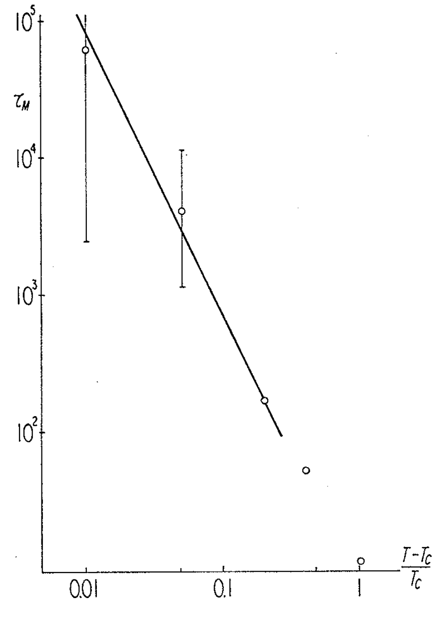

Fig. 1. The log-log plots of relaxation time of polarization versus $(T-T_c)/T_c$ which was obtained by a computer simulation.[3] The straight line with gradient -2 is approximately fitted by the three points near T_c rather than near $2T_c$.

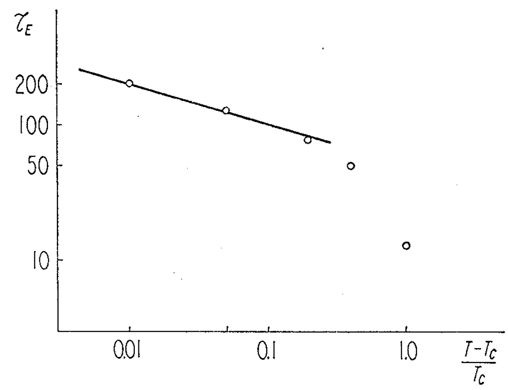

Fig. 2. The log-log plots of relaxation time of energy versus $(T-T_c)/T_c$ which was also obtained by a computer simulation.[3] The straight line with gradient $-\frac{1}{4}$ is approximately fitted by three points near T_c.

can say only that these results are not inconsistent with those obtained by the high temperature expansion and with the similarity law.

§ 6. Summary and discussion

Starting from the Kubo linear response theory, we have formulated the relaxation time and connected it with the dynamical susceptibility in ergodic systems. It has been shown that the relaxation time is proportinal to the corresponding susceptibility (or the canonical correlation function) in some severe conditions. It was argued with the use of an exactly soluble model on linear spin chains that the critical index of slowing down is different from that of the static susceptibility and that there is a possibility that the similarity law holds in this system.

According to Tomita's formulation,[23] the Fourier transform $X_{AA}(q,\omega)$ of the canonical correlation $(A_q^*, A_q(t))$ is expressed by

$$X_{AA}(q,\omega)/\chi(q,0) = 1/\{i\omega+\gamma(q,\omega)\}, \tag{6·1}$$

where

$$\gamma(q,\omega) = X_{\dot{A}\dot{A}}(q,\omega)/\chi(q,0), \tag{6·2}$$

and $X_{\dot{A}\dot{A}}(q,\omega)$ is the force correlation for the quantity A. In particular, if we put $\omega=0$ in Eq. (6·2), the relaxation time τ_A is given by

$$\tau_A = \frac{1}{\gamma(q,0)}. \tag{6·3}$$

That is, the force correlation is equal to

$$X_{\dot{A}\dot{A}}(q,0) = \beta R_A(T). \tag{6·4}$$

Although the function $X_{\dot{A}\dot{A}}(q,0)$ is of the same type as Eq. (3·13), usually the Hermitian conjugate A_q^* does not commute with A_q for $q\neq 0$, and consequently, the time integral of the canonical correlation function, $X_{\dot{A}\dot{A}}(q,0)$ never vanishes for $q\neq 0$. In the isotropic Heisenberg model, the anomalous behavior of $X_{\dot{A}\dot{A}}$ or $R_A(T)$ has been pointed out by Tomita.[23] His results show that the part $X_{\dot{A}\dot{A}}$ or $R_A(T)$ causes kinetic *speeding up*.

According to our expression (3·44) for the relaxation time τ_A, the kinetic speeding up (or the divergence of $R_A(\xi)$ at ξ_c) is brought about, for example, in the case when all the coefficients $\lambda_n(\xi)$ vanish as the parameter ξ approaches the critical value ξ_c. In stochastic models, the first moment λ_1 $(=\mu_1)$, at least, does not vanish even at the critical point. In fact, the non-divergence of $R(\xi)$ at ξ_c can be proved generally in the same way as in a previous paper[2] or on the basis of variational principle.[12),24] That is, in contrast with the isotropic Heisenberg model, not kinetic speeding up but kinetic slowing down occurs in stochastic models.

According to Mori's theory,[8] the relaxation time τ_A is given by

$$\tau_A = \Xi[0] = \frac{1}{\varphi[0]} = (A, A) / \int_0^\infty (f_A(t), f_A)\, dt\,, \tag{6·5}$$

where the variable f_A is a random force defined by

$$f_A(t) = u(t) f_A\,, \qquad f_A = (1-P)\dot{A}\,,$$
$$u(t) = \exp[t(1-P)i\mathcal{L}] \tag{6·6}$$

and

$$PG = (G, A) \cdot (A, A)^{-1} A\,. \tag{6·7}$$

That is, we find that

$$R_A(T) = \frac{1}{\beta} \int_0^\beta (f_A(t), f_A)\, dt\,. \tag{6·8}$$

One of the merits in Mori's theory is the use of a continued-fraction expansion of the time correlation function $(f(t), f)$. It is, in general, expected that the convergence[25] of the continued fraction expansion is better than that of moment expansion. The investigation on the convergence and on the singularity of the continued-fraction, however, is a very difficult problem, and it will be instructive to study the continued-fraction expansion in such an exactly soluble model as discussed in the present paper.

The study on the wave-number dependent relaxation time $\tau(q)$ near the critical point will be an important problem in the future in connection with the dynamical scaling law.[26]

Acknowledgement

The author should like to thank H. Yahata for useful discussions on the kinetic Ising model.

References

1) R. Kubo, J. Phys. Soc. Japan **12** (1957), 570.
2) M. Suzuki, H. Ikari (Yahata) and R. Kubo, *Proceedings of the International Conference on Statistical Mechanics* (Supplement to J. Phys. Soc. Japan **26** (1969)), p. 153.
H. Yahata and M. Suzuki, J. Phys. Soc. Japan **27** (1969), 1421.
3) N. Ogita, A. Ueda, T. Matsubara, H. Matsuda and F. Yonezawa, *Proceedings of the International Conference on Statistical Mechanics* (Supplement to J. Phys. Soc. Japan **26** (1969)), p. 145.
4) R. Kubo, *Statistical Mechanics of Equilibrium and Nonequilibrium*, ed. J. Meixner (Amsterdam, North-Holland), p. 80.
5) R. Kubo, J. Phys. Soc. Japan **17** (1962), 1100.
6) M. Suzuki and R. Kubo, J. Phys. Soc. Japan **24** (1968), 51.
7) K. Kawasaki, Prog. Theor. Phys. **39** (1968), 1133; **40** (1968), 11, 706, 930.
8) H. Mori, Prog. Theor. Phys. **33** (1965), 423; **34** (1965), 399.
9) R. Kubo, Rep. Prog. Phys. **24** (1966), 255.
10) R. Abe, Prog. Theor. Phys. **39** (1968), 947.

11) R. J. Glauber, J. Math. Phys. **4** (1963), 294.
N. Matsudaira, Can. J. Phys. **45** (1967), 2091; J. Phys. Soc. Japan **23** (1967), 232.
K. Kawasaki and T. Yamada, Prog. Theor. Phys. **39** (1968), 1.
K. Yoshimitsu and T. Matsubara, Prog. Theor. Phys. Suppl. Extra Number (1968), 109.
H. Mamada and F. Takano, J. Phys. Soc. Japan **25** (1968), 675.
T. Obokata, J. Phys. Soc. Japan **26** (1969), 895.
12) R. Abe and A. Hatano, Prog. Theor. Phys. **41** (1969), 941.
13) E. Lieb, T. Schultz and D. Mattis, Ann. of Phys. **16** (1961), 407.
S. Katsura, Phys. Rev. **127** (1962), 1508; **129** (1963), 2835.
M. Suzuki, J. Phys. Soc. Japan **21** (1966), 2140.
14) S. A. Pikin and V. M. Tsukernik, Soviet Phys.—JETP **23** (1966), 914.
15) Th. Niemeijer, Physica **36** (1967), 377; **39** (1968), 313.
16) S. Katsura, T. Horiguchi and M. Suzuki, Physica **45** (1970), No. 5.
17) T. Oguchi and I. Ono, J. Phys. Soc. Japan **26** (1969), 1378.
The two-dimensional case was discussed in the following papers.
M. E. Fisher, J. Math. Phys. **4** (1963), 124.
T. Obokata, I. Ono and T. Oguchi, J. Phys. Soc. Japan **23** (1967), 516.
G. A. T. Allan and D. D. Betts, Can. J. Phys. **46** (1968), 15.
D. D. Betts and M. H. Lee, Phys. Rev. Letters **20** (1968), 1507.
18) H. Falk, Phys. Rev. **165** (1968), 602.
19) R. M. Wilcox, Phys. Rev. **174** (1968), 624.
20) G. S. Rushbrooke, J. Chem. Phys. **39** (1963), 842.
M. E. Fisher, J. Math. Phys. **5** (1964), 944.
R. B. Griffiths, J. Chem. Phys. **43** (1965), 1958.
21) B. Widom, J. Chem. Phys. **43** (1965), 3839.
C. Domb and D. L. Hunter, Proc. Phys. Soc. **86** (1965), 1147.
A. Z. Patashinsky and V. L. Pokrovsky, Soviet Phys.—JETP **50** (1966), 439.
L. P. Kadanoff, Physics **2** (1966), 263.
M. Suzuki, Prog. Theor. Phys. **38** (1967), 289, 744, 1225; **39** (1968), 349.
R. Abe, Prog. Theor. Phys. **38** (1967), 72.
22) M. E. Fisher, Physica **25** (1959), 521; **28** (1962), 172; J. Math. Phys. **5** (1964), 944.
L. P. Kadanoff, Nuovo Cim. **44** (1966), 276.
23) K. Tomita, Japan Atomic Energy Research Institute **1113** (1966), 106; **1157** (1968), 80.
K. Tomita and T. Kawasaki, *Proceedings of the International Conference on Statistical Mechanics* (Supplement to J. Phys. Soc. Japan **26** (1969)), p. 157.
24) K. Kawasaki, Phys. Rev. **143** (1966), 375.
L. P. Kadanoff and J. Swift, Phys. Rev. **165** (1968), 310.
25) H. S. Wall, *Analytic Theory of Continued Fractions* (Chelsea Pub. Co., Bronx, N. Y., 1967).
26) B. I. Halperin and P. C. Hohenberg, Phys. Rev. Letters **19** (1967), 700; Phys. Rev. **177** (1969), 952.
H. Mori and H. Okamoto, Prog. Theor. Phys. **40** (1968), 1287.

Note added in Proof:

Quite recently, I. Hatta has found experimental data on dielectric relaxation time near the transition points in $NaNO_2$ (to be published in J. Phys. Soc. Japan), which seem to support our theoretical prediction that the critical index of the relaxation time is larger than that of the static susceptibility in the stochastic Ising model.