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Fluctuation, Relaxation, and Extensivity of Macrovariables in Nonequilibrium Systems

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The extensive property of a macrovariable is proved for a quantal system whose Hamiltonian depends on time and for a stochastic system whose temporal evolution operator depends on time. These generalized situations are concerned with bulk-contact open systems. The extensive property, fluctuation, and nonlinear relaxation are investigated explicitly by calculating rigorously generating functions in exactly soluble models such as the linear stochastic model and linear *XY* model. The relation between the nonlinear critical slowing down and linear critical slowing down is also discussed.

KEY WORDS: Nonlinear relaxation and fluctuation; extensive property of macrovariable; bulk-contact open system; generating function; stochastic model; *XY* model; exact solution; critical slowing down; existence of thermodynamic limit.

1. INTRODUCTION

Recently van Kampen[1] and Kubo *et al.*[2–4] developed asymptotic evaluation methods for investigating the fluctuation and relaxation of a macrovariable. In particular, Kubo[2–4] proposed the extensivity Ansatz that the distribution

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function of $P(X, t)$ of an extensive macrovariable X at time t has the asymptotic form

$$P(X, t) = C \exp[\Omega\phi(x, t)] \tag{1}$$

for a large system size Ω, with $x = X/\Omega$. This is a generalization of the concept of the extensive property of equilibrium statistical thermodynamics to nonequilibrium problems and it has been found to be very useful in discussing fluctuation and relaxation of a macrovariable. In Refs. 5–8 Kubo's extensivity Ansatz has been proven under general conditions. That is, the extensivity Ansatz has been proven in Ref. 6 (hereafter referred to as I) to hold in microscopic stochastic systems and quantum mechanical systems, under the conditions that the initial distribution ρ_0 has the form

$$\rho_0 = C_0 \exp \mathscr{H}^{(i)}; \qquad \mathscr{H}^{(i)} = \int \mathscr{H}^{(i)}(\mathbf{r})\, d\mathbf{r} \tag{2}$$

and that the relevant macrovariable X and the Hamiltonian $\mathscr{H}$ are sums of the forms

$$X = \int X(\mathbf{r})\, d\mathbf{r} \qquad \text{and} \qquad \mathscr{H} = \int \mathscr{H}(\mathbf{r})\, d\mathbf{r} \tag{3}$$

respectively, where the local operators $\mathscr{H}^{(i)}(\mathbf{r})$, $X(\mathbf{r})$, and $\mathscr{H}(\mathbf{r})$ are *bounded* in the sense of certain canonical averages.[6] In I, the Hamiltonian of a quantal system has been assumed, for simplicity, to change suddenly only at the initial time and the temporal evolution operator Γ of a stochastic system has been assumed to be time independent. One of our purposes in this paper is to extend the proof of I to more general cases in which the Hamiltonian $\mathscr{H}$ and temporal evolution operator Γ depend on time t. Another purpose is to give some examples in which the extensive property can be shown explicitly by calculating exactly the generating functions of the relevant macrovariables introduced in I. In Ref. 7 (hereafter referred to as II) we have proved the extensivity of a *Markovian* macrovariable on the basis of the master equation, by the use of the mean value theorem in differential calculus, and obtained the following asymptotic equation for the generating function:

$$\frac{\partial}{\partial t}\psi(\lambda, t) + \mathscr{H}\left(\frac{\partial\psi}{\partial\lambda}, -\lambda, t\right) = 0 \tag{4}$$

where the master equation is written in the form

$$\epsilon\frac{\partial}{\partial t}P(x, t) + \mathscr{H}\left(x, \epsilon\frac{\partial}{\partial x}, t\right)P(x, t) = 0 \tag{5}$$

with $\epsilon = 1/\Omega$, and the generating function $\Psi(\lambda, t)$ takes the form

$$\Psi(\lambda, t) \equiv \int P(X, t)e^{\lambda X}\, dX \cong C \exp[\Omega\psi(\lambda, t)] \tag{6}$$

By the help of the above asymptotic equation (4) of the generating function, the expressions[1-4] of temporal evolution of the most probable path $y(t)$, variance $\sigma(t)$, and other fluctuations around $y(t)$ have been rederived in II:

$$\dot{y}(t) = c_1(y(t), t), \qquad \dot{\sigma}(t) = 2c_1'(y(t), t)\sigma(t) + c_2(y(t), t) \tag{7}$$

where $c_n(x, t)$ is the nth moment of the intensive transition probability defined through

$$\mathscr{H}(x, p, t) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n!} c_n(x, t)p^n \tag{8}$$

We have also discussed in II how the system approaches the equilibrium state in the above framework of the asymptotic evaluation of the distribution function.

In Section 2, the extensivity Ansatz is proved for a quantal system described by the time-dependent Hamiltonian $\mathscr{H}(t)$ under conditions similar to those in I. In Section 3, the extensivity Ansatz is proved for a stochastic system with a time-dependent temporal evolution operator $\Gamma(t)$, under the condition that the system is "normal," as in I. Some exactly soluble examples are given in appendices.

2. EXTENSIVE PROPERTY IN QUANTAL SYSTEMS

As in I and II, it is convenient to make use of a generating function defined by

$$\Psi(\lambda, t) = \begin{cases} \mathrm{Tr}[\exp(\lambda \mathbf{X})]\rho(t) & \text{(quantal)} \\ \sum_{\text{config}} [\exp(\lambda \mathbf{X})]P(t) & \text{(stochastic or classical)} \end{cases} \tag{9}$$

where $\rho(t)$ and $P(t)$ denote the density matrix of a quantal system and the probability distribution function of a stochastic (or classical) system, respectively. If the generating function is proved to have the extensive property, i.e., $\Psi(\lambda, t) = C_1 \exp[\Omega\psi(\lambda, t)]$ for large Ω, then the distribution function $P(X, t)$ of a macrovariable X and the reduced density matrix $\rho(X, t)$, which are, respectively, defined by[6]

$$P(X, t) = \sum \delta(\mathbf{X} - X)P(t), \qquad \rho(X, t) = \mathrm{Tr}\, \delta(\mathbf{X} - X)\rho(t) \tag{10}$$

are shown[6] to take the following asymptotic forms (i.e., extensive properties)

$$P(X, t) \text{ or } \rho(X, t) = C \exp[\Omega\phi(x, t)] \tag{11}$$

by the inverse transformation

$$P(X, t) \text{ or } \rho(X, t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{-\lambda X}\Psi(\lambda, t)\, d\lambda \qquad (12)$$

The function $\phi(x, t)$ is given by the relation

$$\phi(x, t) = \psi(\lambda_0, t) - \lambda_0 x; \qquad \partial\psi(\lambda_0, t)/\partial\lambda_0 = x \qquad (13)$$

Now we assume (2) and (3) with a time-dependent local Hamiltonian $\mathscr{H}(\mathbf{r}, t)$. Then we can prove the following theorem.

Theorem 1. If the local operators $\mathbf{X}(\mathbf{r})$, $\mathscr{H}^{(i)}(\mathbf{r})$, and $\mathscr{H}(\mathbf{r}, t)$ are bounded in averages defined later, then we obtain

$$\lim_{\Omega\to\infty} \Omega^{-1} \log \Psi(\lambda, t) \equiv \lim_{\Omega\to\infty} \psi_\Omega(\lambda, t) = \psi(\lambda, t) \text{ (uniformly convergent)} \qquad (14)$$

for $|\lambda| \leqslant \Lambda$ (fixed) and finite t. Therefore, $\Psi(\lambda, t)$ has the extensive property and consequently so does $\rho(X, t)$.

In order to prove Theorem 1, we consider systems of increasing size L_n (say, $L_n = 2^n a$, where n is a large integer and $\Omega_n = L_n{}^d$), as in I. (See Fig. 1.) Correspondingly, we define $\psi_n(\lambda, t)$ by

$$\psi_n(\lambda, t) = \Omega_n^{-1} \log \Psi_{\Omega_n}(\lambda, t) \qquad (15)$$

where $\Psi_{\Omega_n}(\lambda, t)$ is the generating function for the system size Ω_n. As in I, our main task is to prove that this series of functions $\{\psi_n(\lambda, t)\}$ satisfies Cauchy's condition on convergence. For this purpose, we divide the volume Ω_n into 2^d subdomains Ω_{n-1} and provide each domain with an inside margin of width b (the range of local operators) as shown in Fig. 2. Each margined domain of Ω_{n-1} is denoted by $\hat{\Omega}_{n-1}$ (i.e., the volume $\hat{\Omega}_n = \hat{L}_n{}^d$; $\hat{L}_n = L_n - 2b$). Thus, we redefine $\Psi_{\Omega_n}(\lambda, t)$ by (9) with $\mathbf{X}$, $\mathscr{H}^{(i)}$, and $\mathscr{H}(t)$ defined by integrals (2) and (3) over the domain $\hat{\Omega}_n$. For the precise definition of local

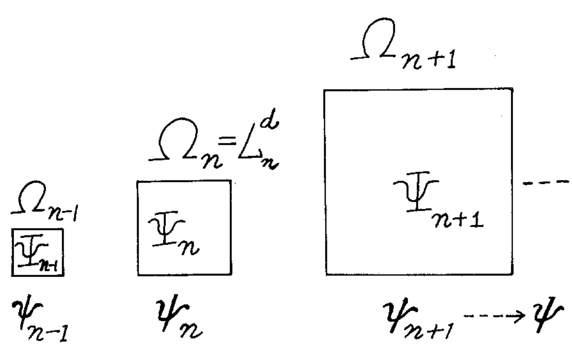

Fig. 1. A series of systems with increasing size L_n and an associated series of ψ_n.

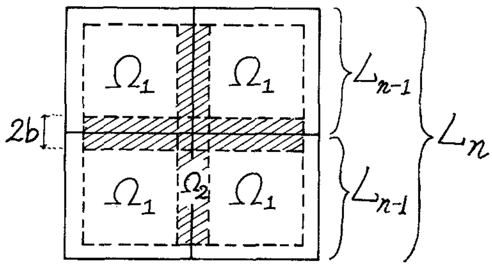

Fig. 2. Domains Ω_1 with inside margins of width b; Ω_2 is the shaded region.

operators, see I. Let us call the boundary region shaded in Fig. 2 domain Ω_2 and the rest we call domain Ω_1. That is, $\hat{\Omega}_n = \Omega_1 + \Omega_2$. Then, we separate each of the operators $\mathbf{X}$, $\mathscr{H}^{(i)}$, and $\mathscr{H}(t)$ into two parts:

$$\mathbf{X} = \mathbf{X}_1 + \mathbf{X}_2, \qquad \mathscr{H}^{(i)} = \mathscr{H}_1^{(i)} + \mathscr{H}_2^{(i)}, \qquad \mathscr{H}(t) = \mathscr{H}_1(t) + \mathscr{H}_2(t) \tag{16}$$

where

$$\mathbf{X}_j = \int_{\Omega_j} \mathbf{X}(\mathbf{r})\, d\mathbf{r}, \qquad \mathscr{H}_j^{(i)} = \int_{\Omega_j} \mathscr{H}^{(i)}(\mathbf{r})\, d\mathbf{r}, \qquad \mathscr{H}_j(t) = \int_{\Omega_j} \mathscr{H}(\mathbf{r}, t)\, d\mathbf{r} \tag{17}$$

Now, as in I, one of the key points for the proof of the existence of the thermodynamic limit is to evaluate the difference between the two generating functions corresponding to $\Omega_1 + \Omega_2$ and Ω_1 as follows:

$$|\log \Psi_{\Omega_1+\Omega_2}(\lambda, t) - \log \Psi_{\Omega_1}(\lambda, t)| \leqslant \epsilon_n(\lambda, t) \tag{18}$$

Here, the upper bound $\epsilon_n(\lambda, t)$ is expressed by $\epsilon_n(\lambda, t) = \epsilon_1 + \epsilon_2 + \epsilon_3$, and

$$\begin{aligned}
\epsilon_1 &\equiv |\log \Psi_{\Omega_1+\Omega_2} - \log \mathrm{Tr}[\exp(\lambda \mathbf{X}_1)]\rho(t)| \\
\epsilon_2 &\equiv |\log \mathrm{Tr}[\exp(\lambda \mathbf{X}_1)]\rho(t) - \log \mathrm{Tr}[\exp(\lambda \mathbf{X}_1)]U(t)(\exp \mathscr{H}_1^{(i)})U^\dagger(t)| \\
\epsilon_3 &\equiv |\log \mathrm{Tr}[\exp(\lambda \mathbf{X}_1)]U(t)(\exp \mathscr{H}_1^{(i)})U^\dagger(t) - \log \Psi_{\Omega_1}|
\end{aligned} \tag{19}$$

where $\rho(t)$ is determined by the Liouville equation

$$i\frac{\partial \rho(t)}{\partial t} = [\mathscr{H}(t), \rho(t)]; \qquad \hbar = 1 \tag{20}$$

The formal solution is given by[9-11]

$$\begin{aligned}
\rho(t) &= \exp_+\left\{\frac{1}{i}\int_0^t \mathscr{H}^\times(t')\, dt'\right\}\rho(0) \\
&= \rho(0) + \sum_{n=1}^{\infty} \left(\frac{1}{i}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n\, \mathscr{H}^\times(t_1) \cdots \mathscr{H}^\times(t_n)\rho(0)
\end{aligned} \tag{21}$$

with Kubo's notation $A^\times B = [A, B]$, or

$$\rho(t) = U(t)\rho(0)U^\dagger(t) \tag{22}$$

where

$$U(t) = \exp_+\left\{\frac{1}{i}\int_0^t \mathscr{H}(t')\,dt'\right\}$$
$$= 1 + \sum_{n=1}^{\infty}\left(\frac{1}{i}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n\, \mathscr{H}(t_1)\cdots\mathscr{H}(t_n) \tag{23}$$

For the details of the ordered exponential $\exp_+(\cdots)$, see the paper by Kubo.[12] In particular, we have

$$U^\dagger(t) = \exp_-\left\{\frac{1}{i}\int_0^t \mathscr{H}(t')\,dt'\right\}$$
$$= 1 + \sum_{n=1}^{\infty}\left(\frac{1}{i}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} \mathscr{H}(t_n)\cdots\mathscr{H}(t_1) \tag{24}$$

and

$$\frac{\partial U(t)}{\partial \lambda} = \frac{1}{i}\, U(t)\int_0^t dt'\, U^\dagger(t')\,\frac{\partial \mathscr{H}(t')}{\partial \lambda}\, U(t') \tag{25}$$

Equation (25) will be used frequently in this paper. The main difference of the present treatment from that in I is the use of $U(t)$ given by (23) instead of $\exp(-it\mathscr{H})$ in evaluating the upper bound $\epsilon_n(\lambda, t)$ in (18). The quantity ϵ_1 is rewritten as follows:

$$\epsilon_1 = \left|\int_2^1 \frac{d}{d\mu}\log \operatorname{Tr}\{\exp \lambda(\mathbf{X}_1 + \mu\mathbf{X}_2)\}\rho(t)\,d\mu\right| \tag{26}$$

As shown in I, the following formula holds.

$$\frac{d}{dx}\, e^{A+xB} = \int_0^1 e^{(1-s)(A+xB)} B e^{s(A+xB)}\,ds = \int_0^1 e^{s(A+xB)} B e^{(1-s)(A+xB)}\,ds \tag{27}$$

It is convenient to define, as in I, the following operation (or mapping) $P_{(s,\mu)}$ associated with an operator P:

$$P_{(s,\mu)}Q \equiv e^{-s(P_1+\mu P_2)} Q e^{s(P_1+\mu P_2)} \tag{28}$$

where the operators P_1 and P_2 are defined by

$$P_j = \int_{\Omega_j} P(\mathbf{r})\,d\mathbf{r} \tag{29}$$

Then, ϵ_1 is written as

$$\epsilon_1 = \left|\lambda\int_0^1 d\mu \int_0^1 ds\, \operatorname{Tr}(\mathbf{X}_{(-s,\mu)}\mathbf{X}_2)\{\exp[\lambda(\mathbf{X}_1 + \mu\mathbf{X}_2)]\}\rho(t)\right| Z_{\lambda,\mu}^{-1} \tag{30}$$

where

$$Z_{\lambda,\mu} = \mathrm{Tr}\,\exp[\lambda(\mathbf{X}_1 + \mu\mathbf{X}_2)]\rho(t) \tag{31}$$

By the use of the property that

$$\mathrm{Tr}[(P_{(-s,\mu)}A)\cdot B] = \mathrm{Tr}[AP_{(s,\mu)}B] \tag{32}$$

we obtain

$$\epsilon_1 = \left|\lambda\int_0^1 d\mu\int_0^1 ds\int_{\Omega_2} d\mathbf{r}\langle\mathbf{X}(\mathbf{r})\rangle^{(1)}\right| \leqslant (|\lambda|c_1)\Omega_2 \tag{33}$$

where the average $\langle\cdots\rangle^{(1)}$ is defined by

$$\langle\mathbf{X}\rangle^{(1)} \equiv \mathrm{Tr}\,\mathbf{X}\rho_1/\mathrm{Tr}\,\rho_1; \qquad \rho_1 \equiv \{\exp[\lambda(\mathbf{X}_1 + \mu\mathbf{X}_2)]\}\mathbf{X}_{(s,\mu)}\rho(t) \tag{34}$$

and we have assumed that

$$|\langle\mathbf{X}\rangle^{(1)}| \leqslant c_1 \qquad \text{(bounded)} \tag{35}$$

In a similar way, we get

$$\begin{aligned}\epsilon_2 &= |\log\mathrm{Tr}(\exp\lambda\mathbf{X}_1)\rho(t) - \log\mathrm{Tr}(\exp\lambda\mathbf{X}_1)U(t)(\exp\mathscr{H}_1^{(i)})U^\dagger(t)| \\ &= \left|\int_0^1 d\mu\frac{d}{d\mu}\log\mathrm{Tr}\{U^\dagger(t)(\exp\lambda\mathbf{X}_1)U(t)\}\exp\{\mathscr{H}_1^{(i)} + \mu\mathscr{H}_2^{(i)}\}\right| \\ &= Z_2^{-1}\left|\int_0^1 d\mu\int_0^1 ds\,\mathrm{Tr}\{U^\dagger(t)(\exp\lambda\mathbf{X}_1)U(t)\}\right. \\ &\quad\left.\times\exp s(\mathscr{H}_1^{(i)} + \mu\mathscr{H}_2^{(i)})\mathscr{H}_2^{(i)}\exp(1-s)(\mathscr{H}_1^{(i)} + \mu\mathscr{H}_2^{(i)})\right|\end{aligned} \tag{36}$$

where we have used Eq. (27), and

$$Z_2 = \mathrm{Tr}\,U^\dagger(t)(\exp\lambda\mathbf{X}_1)U(t)\exp(\mathscr{H}_1^{(i)} + \mu\mathscr{H}_2^{(i)}) \tag{37}$$

Thus, we obtain

$$\epsilon_2 = Z_2^{-1}\left|\int_0^1 d\mu\int_0^1 ds\,\mathrm{Tr}\,\mathscr{H}_2^{(i)}\exp(\mathscr{H}_1^{(i)} + \mu\mathscr{H}_2^{(i)})\exp[\lambda\mathscr{H}_{(s,\mu)}^{(i)}U^\dagger(t)\mathbf{X}_1U(t)]\right. \tag{38}$$

with the notation (28). Here we define an average $\langle\cdots\rangle^{(2)}$ by

$$\begin{gathered}\langle\mathscr{H}_2^{(i)}\rangle^{(2)} = \mathrm{Tr}\,\mathscr{H}_2^{(i)}\rho_2/\mathrm{Tr}\,\rho_2 \\ \rho_2 \equiv \exp[\mathscr{H}_1^{(i)} + \mu\mathscr{H}_2^{(i)}]\exp[\lambda\mathscr{H}_{(s,\mu)}^{(i)}U^\dagger(t)\mathbf{X}_1U(t)]\end{gathered} \tag{39}$$

Then, assuming that $|\langle\mathscr{H}_2^{(i)}(\mathbf{r})\rangle^{(2)}| \leqslant c_2$ (finite), we get

$$\epsilon_2 = \left|\int_0^1 d\mu\int_0^1 ds\int_{\Omega_2} d\mathbf{r}\,\langle\mathscr{H}_2^{(i)}(\mathbf{r})\rangle^{(2)}\right| \leqslant c_2\Omega_2 \tag{40}$$

Finally, ϵ_3 is evaluated as follows. First note that ϵ_3 is given by

$$\epsilon_3 = \left| \int_0^1 d\mu \frac{d}{d\mu} \log \operatorname{Tr}(\exp \lambda \mathbf{X}_1) U_\mu(t)(\exp \mathscr{H}_1^{(i)}) U_\mu{}^\dagger(t) \right| \tag{41}$$

where

$$U_\mu(t) \equiv \exp_+ \left[(1/i) \int_0^t \{\mathscr{H}_1(t') + \mu \mathscr{H}_2(t')\}\, dt' \right] \tag{42}$$

Consequently, we have

$$\epsilon_3 \leqslant \epsilon_{3,1} + \epsilon_{3,2} \tag{43}$$

where

$$\begin{aligned} \epsilon_{3,1} &= \left| \int_0^1 d\mu \operatorname{Tr}(\exp \lambda \mathbf{X}_1) \left[\frac{d}{d\mu} U_\mu(t) \right] (\exp \mathscr{H}_1^{(i)}) U_\mu{}^\dagger(t) \right| Z_3^{-1} \\ \epsilon_{3,2} &= \left| \int_0^1 d\mu \operatorname{Tr}(\exp \lambda \mathbf{X}_1) U_\mu(t)(\exp \mathscr{H}_1^{(i)}) \frac{d}{d\mu} U_\mu{}^\dagger(t) \right| Z_3^{-1} \end{aligned} \tag{44}$$

and

$$Z_3 = \operatorname{Tr}(\exp \lambda \mathbf{X}_1) U_\mu(t)(\exp \mathscr{H}_1^{(i)}) U_\mu{}^\dagger(t) \tag{45}$$

By the help of formula (25), we obtain

$$\epsilon_{3,1} = \left| \int_0^1 d\mu \int_0^t dt' \int_{\Omega_2} d\mathbf{r}\, \langle \mathscr{H}(\mathbf{r}, t') \rangle^{(3)} \right| \leqslant t c_3 \Omega_2 \tag{46}$$

under the condition that $|\langle \mathscr{H}(\mathbf{r}, t')\rangle^{(3)}| \leqslant c_3$, where the average $\langle \cdots \rangle^{(3)}$ is defined by

$$\begin{aligned} \langle \mathscr{H}(\mathbf{r}, t') \rangle^{(3)} &= \operatorname{Tr} \mathscr{H}(\mathbf{r}, t') \rho_3 / \operatorname{Tr} \rho_3 \\ \rho_3 &= U_\mu(t')(\exp \mathscr{H}_1^{(i)}) U_\mu{}^\dagger(t)(\exp \lambda \mathbf{X}_1) U_\mu(t) U_\mu{}^\dagger(t') \\ &= \exp[U_\mu(t') \mathscr{H}_1^{(i)} U_\mu{}^\dagger(t')] \exp[\lambda U_\mu(t') U_\mu{}^\dagger(t) \mathbf{X}_1 U_\mu(t) U_\mu{}^\dagger(t')] \end{aligned} \tag{47}$$

Similarly, $\epsilon_{3,2}$ is given by

$$\epsilon_{3,2} = \left| \int_0^1 d\mu \int_0^t dt' \int_{\Omega_2} d\mathbf{r}\, \langle \mathscr{H}(\mathbf{r}, t') \rangle^{(4)} \right| \tag{48}$$

where

$$\langle \mathscr{H}(\mathbf{r}, t') \rangle^{(4)} = \operatorname{Tr} \mathscr{H}(\mathbf{r}, t') \rho_3{}^\dagger / \operatorname{Tr} \rho_3{}^\dagger \tag{49}$$

Then we get $|\langle \mathscr{H}(\mathbf{r}, t') \rangle^{(4)}| \leqslant c_3$. Consequently, we obtain

$$\epsilon_{3,2} \leqslant t c_3 \Omega_2 \tag{50}$$

Thus we arrive finally at the inequality

$$\epsilon_n(\lambda, t) \leqslant (|\lambda| c_1 + c_2 + 2 t c_3) \Omega_2 \tag{51}$$

Therefore, Eqs. (15) and (18) with (51) lead to the following inequality:

$$|\psi_n(\lambda, t) - \psi_{n-1}(\lambda, t)| \leqslant 2^{-n}c(t); \qquad c(t) = (\Lambda c_1 + c_2 + 2tc_3)(2bd/a) \tag{52}$$

Here we have made use of the facts that $\Omega_2 = (2bd)L_n^{d-1}$ + higher terms and that $\Omega_n = L_n{}^d = 2^{nd}a^d$. Repeated application of Eq. (52) yields

$$|\psi_{n+m}(\lambda, t) - \psi_n(\lambda, t)| \leqslant 2^{-n}c(t) \qquad \text{for} \quad |\lambda| \leqslant \Lambda \quad \text{(fixed)} \tag{53}$$

and for any positive integer m. This is Cauchy's condition of the uniform convergence of the series $\{\psi_n(\lambda, t)\}$ for t finite (fixed). Hence Theorem 1 holds. The limit $\psi(\lambda, t)$ obtained for the above particular sequence of squares is also obtained for an arbitrary sequence of squares with edge increasing to infinity as in the static proof[13,14] of the thermodynamic limit of free energy.

3. EXTENSIVE PROPERTY IN STOCHASTIC MODELS

In this section we prove the extensivity of the probability distribution function $P(X, t)$ of a macrovariable X. The main procedure of the proof is much the same as for quantal systems. The conditions of the validity for stochastic models are, however, much simplified compared to those of quantal systems. That is, the extensivity of a stochastic model holds under the condition that the microscopic distribution function $P(\{\sigma_j\}, t)$ is "normal" in the sense that

$$P(..., -\sigma_j,..., t) \leqslant C_3 P(..., \sigma_j,..., t); \qquad \sigma_j = \pm 1 \tag{54}$$

for any configuration, where C_3 is a constant independent of the system size Ω. We designate this as $P \in \mathcal{N}$.

As in I, we start from the microscopic master equation

$$(\partial/\partial t)P(\{\sigma_j\}, t) = \Gamma(t)P(\{\sigma_j\}, t) \tag{55}$$

with the following temporal evolution operator of single spin flips; $\Gamma(t) = \sum_j \Gamma(j, t)$ and

$$\Gamma(j, t)P(\{\sigma_j\}, t) = -W_j(\sigma_j, t)P(..., \sigma_j,..., t) + W_j(-\sigma_j, t)P(..., -\sigma_j,..., t) \tag{56}$$

where $W_j(\sigma_j, t)$ denotes the time-dependent transition probability of a spin j. Now, we assume that P_0 is given by $P_0 = \exp \mathscr{H}^{(i)}$ with (2). As in Section 2, we divide the system Ω_n into two parts Ω_1 and Ω_2 to confirm Cauchy's condition (53). Accordingly, $\Gamma(t)$ and $\mathscr{H}(t)$ are separated, respectively, as

$$\Gamma(t) = \Gamma_1(t) + \Gamma_2(t) \qquad \text{and} \qquad \mathscr{H}(t) = \mathscr{H}_1(t) + \mathscr{H}_2(t) \tag{57}$$

Then the following theorem holds with the definition

$$V_\mu(t) \equiv \exp_+ \int_0^t \{\Gamma_1(s) + \mu\Gamma_2(s)\}\, ds \tag{58}$$

Theorem 2 (stochastic). If $\hat{P}(t') \equiv V_\mu(t')P_0 \in \mathcal{N}$ ("normal") for any separation of $\Gamma(t)$ into two parts $\Gamma_1(t)$ and $\Gamma_2(t)$ and for $0 \leqslant t' \leqslant t$ and $0 \leqslant \mu \leqslant 1$, then we have

$$\lim_{\Omega\to\infty} \psi_\Omega(\lambda, t) = \psi(\lambda, t) \qquad \text{(uniformly convergent)} \tag{59}$$

for $-\Lambda \leqslant \lambda \leqslant \Lambda$ (Λ = fixed) and t finite. Therefore, $\Psi(\lambda, t)$ and $P(X, t)$ have the extensive property.

For proof of this theorem, it is sufficient to derive the inequality (18) with $\epsilon_n(\lambda, t) = \epsilon_1 + \epsilon_2 + \epsilon_3 = O(L_n^{d-1})$, where

$$\begin{aligned}
\epsilon_1 &\equiv \left|\log \sum (\exp \lambda\mathbf{X})P(t) - \log \sum (\exp \lambda\mathbf{X}_1)P(t)\right| \\
\epsilon_2 &\equiv \left|\log \sum (\exp \lambda\mathbf{X}_1)P(t) - \log \sum (\exp \lambda\mathbf{X}_1)V_1(t) \exp \mathscr{H}_1^{(i)}\right| \\
\epsilon_3 &\equiv \left|\log \sum (\exp \lambda\mathbf{X}_1)V_1(t) \exp \mathscr{H}_1^{(i)} - \log \sum (\exp \lambda\mathbf{X}_1)V_0(t) \exp \mathscr{H}_1^{(i)}\right|
\end{aligned} \tag{60}$$

(i) Since $\mathbf{X}_1$ commutes with $\mathbf{X}_2$ in the stochastic system, we obtain

$$\epsilon_1 = \left|\int_0^1 d\mu \frac{d}{d\mu} \log \sum [\exp \lambda(\mathbf{X}_1 + \mu\mathbf{X}_2)]P(t)\right| = \left|\lambda \int_0^1 \langle\mathbf{X}_2\rangle_\mu^{(1)}\, d\mu\right| \tag{61}$$

and

$$\langle\mathbf{X}_2\rangle_\mu^{(1)} = \sum \mathbf{X}_2[\exp \lambda(\mathbf{X}_1 + \mu\mathbf{X}_2)]P(t)\Big/\sum [\exp \lambda(\mathbf{X}_1 + \mu\mathbf{X}_2)]P(t) \tag{62}$$

where $\sum$ denotes the sum over all configurations. Clearly, we have

$$|\langle\mathbf{X}_2\rangle_\mu^{(1)}| \leqslant \|\mathbf{X}_2\| \qquad \text{(maximum value of } \mathbf{X}_2) \tag{63}$$

Therefore, we obtain

$$\epsilon_1 \leqslant |\lambda|\, \|\mathbf{X}_2\| = O(L_n^{d-1}) \tag{64}$$

(i) Similarly, since $\mathscr{H}_1^{(i)}$ commutes with $\mathscr{H}_2^{(i)}$, we obtain

$$\epsilon_2 = \left|\int_0^1 d\mu\, \langle\mathscr{H}_2^{(i)}\rangle_\mu^{(2)}\right| \tag{65}$$

where the average $\langle\cdots\rangle_\mu^{(2)}$ is defined by

$$\langle\mathscr{H}_2^{(i)}\rangle_\mu^{(2)} \equiv \sum (\exp \lambda\mathbf{X}_1)V_1(t)\{P(0)\mathscr{H}_2^{(i)}\}Z_2^{-1}; \qquad Z_2 = \sum (\exp \lambda\mathbf{X}_1)V_1(t)P(0) \tag{66}$$

Note that the following lemma holds.

Lemma 1. If $f(\{\sigma_j\}) \leqslant g(\{\sigma_j\})$ for any configuration, then $V_\mu(t)f \leqslant V_\mu(t)g$ for $t \geqslant 0$ and $0 \leqslant \mu \leqslant 1$.

This is easily seen, as in I, from the fact that if $h \geqslant 0$, then $V_\mu(t)h \geqslant 0$. Note also that $|P(0)\mathscr{H}_2^{(i)}| \leqslant |\mathscr{H}_2^{(i)}|P(0)$. Then, applying Lemma 1 to (66), we obtain

$$|\langle \mathscr{H}_2^{(i)} \rangle_{\mu}^{(2)}| \leqslant \|\mathscr{H}_2^{(i)}\| \qquad \text{and thus} \quad \epsilon_2 \leqslant \|\mathscr{H}_2^{(i)}\| \tag{67}$$

quite in the same way as in I.

(iii) Finally we evaluate ϵ_3 as follows

$$\begin{aligned}\epsilon_3 &= \left| \int_0^1 d\mu \frac{d}{d\mu} \log \sum (\exp \lambda \mathbf{X}_1) V_\mu(t) \exp \mathscr{H}_1^{(i)} \right| \\ &= \left| \int_0^1 d\mu \int_0^t dt' \sum (\exp \lambda \mathbf{X}_1) V_\mu(t) V_\mu^\dagger(t') \Gamma_2(t') V_\mu(t') \exp \mathscr{H}_1^{(i)} \right| Z_3^{-1}\end{aligned} \tag{68}$$

where

$$Z_3 = \sum [\exp(\lambda \mathbf{X}_1)] V_\mu(t) \exp \mathscr{H}_1^{(i)} \tag{69}$$

and we have used the formula

$$\frac{\partial}{\partial \mu} V_\mu(t) = V_\mu(t) \int_0^t dt' \; V_\mu^\dagger(t') \Gamma_2(t') V_\mu(t') \tag{70}$$

which is essentially equivalent to (25). Since $\mathscr{H}^{(i)}$ is an effective initial Hamiltonian of short-range interaction, we have $\exp \mathscr{H}^{(i)} \in \mathscr{N}$. Furthermore, we assume that

$$P_\mu(t') \equiv V_\mu(t') \exp \mathscr{H}_1^{(i)} \in \mathscr{N} \tag{71}$$

In order to evaluate ϵ_3 explicitly, we recall the following lemma proved in I.

Lemma 2. If $f(\{\sigma_j\}) \in \mathscr{N}$, then $|\Gamma_2(t')f| \leqslant C_{\Omega_2}(t) f$, where C_{Ω_2} is a constant dependent on Ω_2, and is given by

$$C_{\Omega_2}(t) = (C_4 + 1)\|\Gamma_{\Omega_2}(t)\|; \qquad \|\Gamma_{\Omega_2}(t)\| = \left[\max_{0 \leq t' \leq t} W_k(\sigma_k, t') \right] \Omega_2 \tag{72}$$

with a certain constant C_4.

Applying this lemma to (68), together with (71) and Lemma 1, we obtain.

$$\begin{aligned}\epsilon_3 &\leqslant \left| \int_0^1 d\mu \int_0^t dt' \sum (\exp \lambda \mathbf{X}_1) V_\mu(t) V_\mu^\dagger(t') \cdot C_{\Omega_2}(t) V_\mu(t') \exp \mathscr{H}_1^{(i)} \right| Z_3^{-1} \\ &= t C_{\Omega_2}(t) = t(C_4 + 1)\|\Gamma_{\Omega_2}(t)\|\end{aligned} \tag{73}$$

Here it should be noted in applying Lemma 1 to (68) that

$$V_\mu(t, t') \equiv V_\mu(t)V_\mu^\dagger(t') = \exp_+ \int_{t'}^{t} \{\Gamma_1(s) + \mu\Gamma_2(s)\}\, ds \tag{74}$$

and consequently this has the same property as $V_\mu(t)$ for $t \geqslant t'$. Thus, Lemma 1 is extended to the following:

Lemma 1′. If $f \leqslant g$, then $V_\mu(t, t')f \leqslant V_\mu(t, t')g$ for $t \geqslant t'$.

Thus we arrive finally at the desired inequality

$$\epsilon_n(\lambda, t) \leqslant |\lambda|\, \|\mathbf{X}_2\| + \|\mathscr{H}_2^{(i)}\| + t(C_4 + 1)\|\Gamma_{\Omega_2}(t)\| \doteq O(L_n^{d-1}) \tag{75}$$

Hence Theorem 2 holds, as in Section 2.

Extensions of the above proof to more general stochastic systems such as a two-spin-flip model are straightforward.

4. CONCLUDING REMARKS

We have proved the extensive property of the reduced density matrix $\rho(x, t)$ or the probability distribution function $P(x, t)$ of a macrovariable X under general conditions on the time-dependent Hamiltonian $\mathscr{H}(t)$ and temporal evolution operator $\Gamma(t)$. The present results will be useful for discussing fluctuations in bulk-contact open systems.

The generating function formalism introduced in the course of the proof is very useful in investigating fluctuation and relaxation of a macrovariable for concrete examples. (Such applications are demonstrated in the appendices.) In fact, the most probable path $y(t)$ of $x = X/\Omega$ and variance $\sigma(t)$ are given by

$$y(t) = (\partial\psi/\partial\lambda)_{\lambda=0} \qquad \text{and} \qquad \sigma(t) = (\partial^2\psi/\partial\lambda^2)_{\lambda=0} \tag{76}$$

respectively, for a large Ω, as shown in I.

In Appendix A, we discuss the noninteracting temporal evolution with an arbitrary initial distribution. This is instructive in understanding how the extensivity arises in nonequilibrium systems. The Lee–Yang circle theorem on zeros of partition functions in the complex fugacity plane is extended to a dynamical system. That is, zeros of the generating function $\Psi(\lambda, t)$ lie on the unit circle of the complex $z \equiv e^\lambda$ plane under "ferromagnetic" conditions. In Appendix B, the extensive property is demonstrated explicitly by solving rigorously the linear stochastic chain. An enhancement of fluctuations[2–5] is shown even in this simple model. In Appendix C, the extensive property and nonlinear relaxation are discussed in the generalized XY model in one dimension. It is shown that the nonergodic property appears in this system. The relation between the nonlinear critical slowing down and the linear critical slowing down is also discussed.

APPENDIX A. NONINTERACTING TEMPORAL EVOLUTION AND ARBITRARY INITIAL DISTRIBUTION

(i) The simplest quantal system showing the extensive property may be the following noninteracting spin system:

$$\mathscr{H}_{\text{NI}} = -J \sum_{j=1}^{\Omega} \sigma_j^x, \qquad \mathbf{X} = \sum_{j=1}^{\Omega} \sigma_j^z, \qquad \text{and} \qquad \mathscr{H}^{(i)} = h \sum_{j=1}^{\Omega} \sigma_j^z \tag{A.1}$$

in which the relevant macrovariable is the total magnetization $\mathbf{X}$ and the initial state is sustained by the Zeeman field. This system is trivial, but it may be instructive for understanding our general theory. The generating function $\Psi(\lambda, t)$ is easily shown from (9) to take the form

$$\Psi(\lambda, t) = \exp[\Omega\psi(\lambda, t)] \qquad \text{(exact for any } \Omega) \tag{A.2}$$

where

$$\psi(\lambda, t) = \log\{\cosh \lambda + \sinh \lambda \tanh h \cos(2tJ/\hbar)\} \tag{A.3}$$

The reduced density-matrix $\rho(X, t)$ is given by (11) with the function $\phi(x, t)$ of the form

$$\phi(x, t) = \log\{a(t) \sinh \lambda(x, t) + \cosh \lambda(x, t)\} - x\lambda(x, t) \tag{A.4}$$

where $a(t) = \tanh h \cos(2tJ/\hbar)$ and $\lambda(x, t)$ is the saddle point determined from (13). In our simple system, $\lambda(x, t)$ is solved explicitly and it is given by

$$\lambda(x, t) = \tanh^{-1}\{[x - a(t)]/[1 - a(t)x]\} \tag{A.5}$$

From (76), the average value $y(t)$ and variance $\sigma(t)$ are, respectively, given by

$$y(t) = a(t) \qquad \text{and} \qquad \sigma(t) = 1 - a^2(t) \tag{A.6}$$

These oscillate and do not damp, as it should be, because this system is nonergodic.

(ii) The second simple example is a stochastic model[15–16] with a noninteracting temporal evolution operator Γ but with an arbitrary initial distribution P_0. The generating function $\Psi(\lambda, t)$ of this N-spin system for any arbitrary extensive macrovariable $\mathbf{X} = \sum_j f_j(\{\sigma_j\})$ is given by

$$\Psi(\lambda, t) = \left\langle \exp\left\{ \lambda \left[\sum_j f_j(\{\sigma_j\}) \right]_{\text{irr}} (\sigma_j \to \sigma_j e^{-\alpha t}) \right\} \right\rangle_0 \tag{A.7}$$

where $\langle Q \rangle_0 = \sum_{(\sigma_j = \pm 1)} Q P_0$ and $[\cdots]_{\text{irr}}$ denotes an irreducible expression of $[\cdots]$, in the sense that it does not contain any redundant part such as $\sigma_j \cdot \sigma_j$ or σ_j^3 (which should be reduced to 1 or σ_j). After such reductions, we replace the variable σ_j by $\sigma_j e^{-\alpha t}$ in $[f(\{\sigma_j\})]_{\text{irr}}$, where α is the strength of interaction with the heat bath (i.e., $\Gamma\sigma_j = -\alpha\sigma_j$). It should be remarked that an enhancement of fluctuation[2,3] can occur even in this simplest example for appropriate macrovariables and initial distributions. For example, the variance $\sigma(t)$ of the short-range order $E = \sum_j \sigma_j\sigma_{j+1}$ is given by

$$\sigma_E(t) = 1 + (2e^{-2\alpha t} - 3e^{-4\alpha t}) \tanh K \tag{A.8}$$

in one dimension, where P_0 is assumed to be given by $P_0 = \exp(K \sum \sigma_j\sigma_{j+1})$. This variance $\sigma_E(t)$ shows a peak at $t = t_p = (2\alpha)^{-1} \log 3$. This is a certain kind of enhancement of fluctuation.[2–5]

In general, the variance $\sigma_M(t)$ of the magnetization for this noninteracting Γ is given by

$$\sigma_M(t) = 1 + (\chi_0 - 1)e^{-2\alpha t} \tag{A.9}$$

where $\chi_0 = N^{-1} \sum_{ij} \langle\sigma_j\sigma_j\rangle_0$, while $M(t) = M(0)e^{-\alpha t}$. The generating function of the magnetization $\Psi_M(\lambda, t)$ is expressed as

$$\begin{aligned} \Psi_M(\lambda, t) &= (c^2 - s^2e^{-2\alpha t})^{N/2} \left\langle \exp\left\{h(\lambda, t) \sum_j \sigma_j\right\} \right\rangle_0 \\ h(\lambda, t) &= \frac{1}{2} \log \frac{1 + e^{-\alpha t} \tanh \lambda}{1 - e^{-\alpha t} \tanh \lambda} \end{aligned} \tag{A.10}$$

with $c = \cosh \lambda$ and $s = \sinh \lambda$. From this, we obtain (A.9) with the use of (76). The relaxation of magnetization is given by a single exponential decay as $M(t) = M(0) \exp(-\alpha t)$ and the energy relaxes as $E(t) = \sum_{\langle i,j\rangle} \langle\sigma_i\sigma_j\rangle_0 \times \exp(-2\alpha t)$.

(iii) Here we consider an extension of the Lee–Yang theorem to dynamical systems. Zeros of the generating function $\Psi_M(\lambda, t)$ in (A.10) are easily shown to lie on the unit circle of the complex fugacity plane $z = e^\lambda$ if $\mathscr{H}^{(i)}$ is effectively ferromagnetic, because the ordinary static Lee–Yang theorem[17–23] yields

$$h(\lambda, t) = i\theta \qquad \text{and thus} \quad z^2 = (1 + i\beta)(1 - i\beta)^{-1} \tag{A.11}$$

with $\beta = e^{\alpha t} \tan \theta$. Thus, we have $|z| = 1$ for real time. The present results will be extended to more realistic interacting systems.

APPENDIX B. THE EXTENSIVE PROPERTY AND NONLINEAR RELAXATION IN THE LINEAR STOCHASTIC MODEL

It is convenient for studying fluctuations rigorously in a stochastic model to make use of a state vector representation[24–27] of the form

$$|P(t)\rangle = \sum_{\{\sigma_j = \pm 1\}} P(\{\sigma_j\}, t)|\{\sigma_j\}\rangle; \qquad |\{\sigma_j\}\rangle = \prod_{j=1}^{\otimes} |\sigma_j\rangle_j \tag{B.1}$$

where

$$|\sigma_j\rangle_j = \begin{pmatrix}1\\0\end{pmatrix}_j \quad \text{for} \quad \sigma_j = 1 \qquad \text{and} \qquad |\sigma_j\rangle_j = \begin{pmatrix}0\\1\end{pmatrix}_j \quad \text{for} \quad \sigma_j = -1 \tag{B.2}$$

In this representation, the master equation of the stochastic system is expressed as

$$\frac{\partial}{\partial t}|P(t)\rangle = W|P(t)\rangle \qquad \text{or} \qquad |P(t)\rangle = e^{tW}|P(0)\rangle \tag{B.3}$$

It is also convenient to introduce the vacuum state[24-27] of the form

$$|0\rangle = \rho_{\text{eq}}^{-1/2}|P_{\text{eq}}\rangle = \rho_{\text{eq}}^{1/2}|1\rangle \equiv \rho_{\text{eq}}^{1/2} \sum_{\{\sigma_j=\pm 1\}} |\{\sigma_j\}\rangle \tag{B.4}$$

where ρ_{eq} is a diagonal operator defined by

$$\rho_{\text{eq}} = e^{-\beta\mathscr{H}}/Z, \qquad Z = \operatorname{Tr} e^{-\beta\mathscr{H}}, \qquad \mathscr{H} = \mathscr{H}(\{\sigma_j^z\}), \quad \text{and} \quad W|\rho_{\text{eq}}\rangle = 0 \tag{B.5}$$

Then, the average motion of a diagonal operator A^z is given by

$$\langle A^z\rangle_t = \langle 1|A^z|P(t)\rangle = \langle 0|A^z|\psi(t)\rangle; \qquad |\psi(t)\rangle = \rho_{\text{eq}}^{-1/2}|P(t)\rangle \tag{B.6}$$

The state vector $|\psi(t)\rangle$ is the solution of the equation

$$\frac{\partial}{\partial t}|\psi(t)\rangle = W(\beta)|\psi(t)\rangle; \qquad W(\beta) = \rho_{\text{eq}}^{-1/2} W \rho_{\text{eq}}^{1/2} \tag{B.7}$$

Now the generating function $\Psi(\lambda, t)$ of this stochastic system for a macrovariable $\mathbf{X}$ is written as

$$\begin{aligned}\Psi(\lambda, t) &= \langle 0|(\exp \lambda\mathbf{X})|\psi(t)\rangle \\ &= \langle 0| \exp(\lambda\mathbf{X}) \exp[tW(\beta)] \exp(\beta\mathscr{H} + \mathscr{H}^{(i)})|0\rangle Z Z_0^{-1}\end{aligned} \tag{B.8}$$

with $Z_0 = \operatorname{Tr}\exp \mathscr{H}^{(i)}$. This is a basic expression for the generating function of the macrovariable $\mathbf{X}$ with the initial distribution $\rho_0 = \exp \mathscr{H}^{(i)}$.

As an exactly soluble example, we consider here the nonlinear relaxation of energy in a linear stochastic chain whose Hamiltonian is described by

$$\mathscr{H} = -J \sum_{j=1}^{N} \sigma_j^z \sigma_{j+1}^z \tag{B.9}$$

The initial effective Hamiltonian $\mathscr{H}^{(i)}$ is assumed to be $\mathscr{H}^{(i)} = -\beta_0\mathscr{H}$. That is, the initial state is in equilibrium at a temperature T_0 (i.e., $\beta_0 = 1/k_B T_0$) with the same Hamiltonian $\mathscr{H}$. The relevant energy macrovariable is given by $\mathbf{X} = \mathscr{H}$. The generating function of this system is rewritten[8] as

$$\Psi(\lambda, \mu, t) = \langle 0|e^{\lambda\mathscr{H}} e^{tW(\beta)} e^{\mu\mathscr{H}}|0\rangle \times Z Z_0^{-1}; \qquad \mu = \beta - \beta_0 \tag{B.10}$$

Here, $W(\beta)$ is given by (B.7) with W of the form

$$W = \frac{1}{2}\sum_{j=1}^{N}\{[1 + \tfrac{1}{2}\gamma\sigma_j^z(\sigma_{j-1}^z + \sigma_{j+1}^z)]\sigma_j^z + [\tfrac{1}{2}\gamma\sigma_j^z(\sigma_{j-1}^z + \sigma_{j+1}^z) - 1]\} \quad \text{(B.11)}$$

where γ is defined in (B.13). According to Felderhof,[25–27] the temporal evolution operator $W(\beta)$ is diagonalized[28] in the form

$$W(\beta) = \sum_{0\le q\le \pi} W_q(\beta); \qquad W_q(\beta) = -\lambda_q(\xi_q{}^+\xi_q + \xi_{-q}^+\xi_{-q} - 1) - \alpha \quad \text{(B.12)}$$

in terms of fermion operators $\xi_q{}^+$, ξ_q, where

$$\lambda_q = \alpha(1 - \gamma\cos q), \qquad \gamma = \tanh(2J/k_BT) \quad \text{(B.13)}$$

and α denotes the strength of interaction with the heat bath. It should be remarked that $|0\rangle$ is the vacuum of this representation: $\xi_q|0\rangle = 0$. On the other hand, the Hamiltonian $\mathscr{H}$ becomes[25–27] off-diagonal in this representation as

$$\mathscr{H}_q = -2J[\cos\psi_q(\xi_q{}^+\xi_q + \xi_{-q}^+\xi_{-q} - 1) + i\sin\psi_q(\xi_q{}^+\xi_{-q}^+ + \xi_q\xi_{-q})] \quad \text{(B.14)}$$

where

$$\psi_q = q + \chi_q, \qquad \sin\chi_q = \alpha(\gamma\sin q - \sin^2\varphi\sin 2q)\lambda_q^{-1}; \qquad \sin 2\varphi = \gamma \quad \text{(B.15)}$$

or

$$\cos\psi_q = (\cos q - \gamma)\alpha\lambda_q^{-1} \qquad \text{and} \qquad \sin\psi_q = (1-\gamma^2)^{1/2}(\sin q)\alpha\lambda_q^{-1} \quad \text{(B.16)}$$

Thus, the generating function of the energy $E = \mathscr{H}$ is expressed in the form

$$\Psi(\lambda, \mu, t) = ZZ_0^{-1}\prod_{0\le q\le\pi} f(q, \lambda, \mu, t) \quad \text{(B.17)}$$

where

$$f(q, \lambda, \mu, t) = \langle 0|e^{\lambda\mathscr{H}_q}e^{tW(\beta)}e^{\mu\mathscr{H}_q}|0\rangle \quad \text{(B.18)}$$

Therefore, we obtain the following result:

$$\psi(\lambda, \mu, t) = \lim_{N\to\infty} N^{-1}\log\Psi = \lim_{N\to\infty} N^{-1}\left\{\sum_{0\le q\le\pi} f(q, \lambda, \mu, t) + \log(ZZ_0^{-1})\right\}$$

$$= \frac{1}{2\pi}\int_0^{\pi}\log f(q, \lambda, \mu, t)\,dq + \log\left(\frac{\cosh\beta J}{\cosh\beta_0 J}\right) \quad \text{(B.19)}$$

Thus, the generating function takes the following asymptotic form:

$$\Psi(\lambda, \mu, t) = C\exp[N\psi(\lambda, \mu, t)] \quad \text{(B.20)}$$

for large N. This is our desired extensivity. It is easy to obtain an explicit expression of $\psi(\lambda, \mu, t)$ or $f(q, \lambda, \mu, t)$. From (B.18), (B.12), (B.14), the evaluation of $f(q, \lambda, \mu, t)$ is similar to the calculation of the free energy in the BCS pairing theory.[29] We introduce the following boson operators:

$$b_q^+ = \xi_{-q}^+ \xi_q^+ \qquad \text{and} \qquad b_q^- = \xi_q \xi_{-q} \tag{B.21}$$

In the subspace spanned by the states $|0, 0\rangle$ and $|-q, q\rangle = b_q^+|0, 0\rangle$, we have

$$\xi_q^+\xi_q + \xi_{-q}^+\xi_{-q} = 2b_q^+b_q^- = b_q^z + 1, \qquad b_q^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{matrix} \cdots |-q, q\rangle \\ \cdots |0, 0\rangle \end{matrix}$$

$$i(\xi_q^+\xi_{-q}^+ + \xi_q\xi_{-q}) = b_q^z = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{B.22}$$

It is convenient to transform these Pauli operators into the following new representation:

$$b_q^{z'} = b_q^z \cos\psi_q + b_q^y \sin\psi_q; \qquad (b_q^{z'})^2 = 1 \tag{B.23}$$

Thus, the operators appearing in (B.18) are given by the following matrices:

$$\exp(\mu\mathscr{H}_q) = \exp(-K_\mu b_q^{z'}) = \cosh K_\mu - b_q^{z'} \sinh K_\mu = \begin{pmatrix} c - c_0 s & ics_0 \\ -ics_0 & c + c_0 s \end{pmatrix}$$

$$c_0 = \cos\psi_q, \qquad c = \cosh K_\mu \tag{B.24}$$

$$s_0 = \sin\psi_q, \qquad s = \sinh K_\mu, \qquad K_\mu = 2J\mu$$

$$\exp[tW_q(\beta)]\exp(\alpha t) = \exp(\epsilon_q b_q) = c_q + s_q b_q^z = \begin{pmatrix} c_q + s_q & 0 \\ 0 & c_q - s_q \end{pmatrix} \tag{B.25}$$

$$c_q = \cosh(t\lambda_q), \qquad s_q = -\sinh(t\lambda_q)$$

$$\exp(\lambda\mathscr{H}_q) = \begin{pmatrix} c' - c_0 s' & is_0 s' \\ -is_0 s' & c' + s_0 s' \end{pmatrix} \tag{B.26}$$

$$c' = \cosh K_\lambda, \qquad s' = \sinh K_\lambda, \qquad K_\lambda = 2J\lambda$$

Consequently, the product of the operators appearing in (B.18) is given by

$$e^{\lambda\mathscr{H}_q} e^{tW_q(\beta)} e^{\mu\mathscr{H}_q} = \begin{pmatrix} A_q & B_q \\ C_q & D_q \end{pmatrix} \tag{B.27}$$

where

$$D_q = (c_q - s_q)(c + c_0 s)(c' + c_0 s') + (c_q + s_q)s_0^2 ss', \quad \text{etc.} \tag{B.28}$$

Noting that

$$\langle 0| e^{\lambda\mathscr{H}_q} e^{tW_q(\beta)} e^{\mu\mathscr{H}_q} |0\rangle = D_q \tag{B.29}$$

we obtain

$$f(q, \lambda, \mu, t) = e^{-\alpha t}\{e^{t\lambda_q}(c + s\cos\psi_q)(c' + s'\cos\psi_q) + e^{-t\lambda_q} ss' \sin^2\psi_q\} \tag{B.30}$$

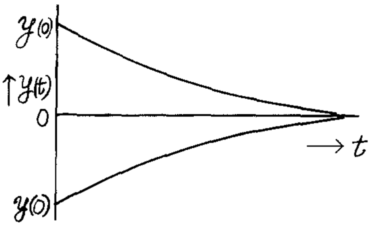

Fig. 3. Relaxation of the energy $y_E(t)$.

Thus, the extensive property is confirmed[8] explicitly in the linear stochastic chain. The nonlinear relaxation of the energy is given by

$$y_E(t) = \langle \mathscr{H} \rangle_t = \left(\frac{\partial \psi}{\partial \lambda}\right)_{\lambda=0} = -J \tanh(\beta J) + \frac{Js}{\pi} \int_0^{\pi} \frac{e^{-2t\lambda_q} \sin^2 \psi_q}{c + s \cos \psi_q} dq \quad \text{(B.31)}$$

This behaves as shown in Fig. 3. The variance $\sigma_E(t)$ is given by the integral

$$\sigma_E(t) = 2J^2 \left[1 - \frac{1}{\pi} \int_0^{\pi} \left\{\cos \psi_q + s \frac{e^{-2t\lambda_q} \sin^2 \psi_q}{c + s \cos \psi_q}\right\}^2 dq\right] \quad \text{(B.32)}$$

It is easily found that the variance $\sigma_E(t)$ shows, in general, an enhancement of fluctuations[2-5] as shown in Fig. 4. In particular, we have

$$\begin{aligned} y_E(0) &= -J \tanh(\beta_0 J), \qquad & y_E(\infty) &= y_{\text{eq}} = -J \tanh(\beta J) \\ \sigma_E(0) &= kT_0 C_v(\beta_0), \qquad & \sigma_E(\infty) &= \sigma_{\text{eq}} = kTC_v(\beta) \end{aligned} \quad \text{(B.33)}$$

where $C_v(\beta)$ denotes the specific heat at the temperature $T\,(=1/k_B\beta)$ and it is given by

$$C_v(\beta) = 2J^2\beta \left[1 - \frac{1}{\pi} \int_0^{\pi} \cos^2 \psi_q \, dq\right] = \frac{2J^2\beta}{\cosh^2(\beta J)} \quad \text{(B.34)}$$

As a special case, we consider a limiting situation in which $T_0 = 0$ and $T = \infty$. The variance of the energy in this limit is given by

$$\sigma_E(t) = \sigma_{\text{eq}} + J^2(2e^{-2\alpha t} - 3e^{-4\alpha t}); \qquad \sigma_{\text{eq}} = J^2 \quad \text{(B.35)}$$

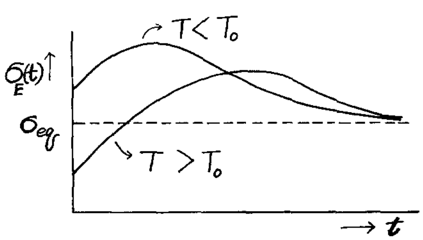

Fig. 4. Time dependence of the variance $\sigma_E(t)$, showing an enhancement of fluctuations.

This shows an enhancement of fluctuations before the system approaches equilibrium. The result (B.35) is consistent with (A.7) for a noninteracting stochastic system. The detailed analyses of the relaxation (B.31) and fluctuation (B.32) for finite T_0 and T will be reported elsewhere.

It seems difficult even in the stochastic chain to obtain in a compact form the generating function of the magnetization

$$\Psi_M(\lambda, t) = \langle 0| \exp(\lambda M) \exp[tW(\beta)] \exp(\beta\mathscr{H} + \mathscr{H}^{(i)})|0\rangle ZZ_0^{-1} \quad \text{(B.36)}$$

because the magnetization cannot be expressed in a bilinear form of fermion operators. The most probable path $y_M(t) = M(t)$ is, however, easily given by

$$M(t) = M(0)e^{-\alpha t} \quad \text{or} \quad M_q(t) = M_q(0)e^{-\lambda_q t} \quad \text{(B.37)}$$

The variance is also easily obtained. For details of fluctuations in the linear region, see Refs. 26 and 27.

APPENDIX C. THE EXTENSIVE PROPERTY IN THE GENERALIZED *XY* MODEL IN ONE DIMENSION

The generalized XY model[28] is described by the Hamiltonian $\mathscr{H} = \mathscr{H}(J_x, J_y, H)$, where

$$\mathscr{H}(J_x, J_y, H) = -\sum_{k=1}^{m}\sum_{j=1}^{N} (J_k{}^x\sigma_j{}^x\sigma_{j+k}^x + J_k{}^y\sigma_j{}^y\sigma_{j+k}^y)\sigma_{j+1}^z \cdots \sigma_{j+k-1}^z + \mu_B H \sum \sigma_j{}^z \quad \text{(C.1)}$$

We assume that the initial Hamiltonian $\mathscr{H}^{(i)}$ is given by

$$\mathscr{H}^{(i)} = -\beta\mathscr{H}(J_x{}^0, J_y{}^0, H^0) \quad \text{(C.2)}$$

Now we are interested in the two macrovariables $\mathbf{X}_1$ and $\mathbf{X}_2$ of the total spin and short-range order:

$$\mathbf{X}_1 = \sum_{j=1}^{N} \sigma_j{}^z, \qquad \mathbf{X}_2 = \sum_{k=1}^{m}\sum_{j=1}^{N} (\sigma_j{}^x\sigma_{j+k}^x + \sigma_j{}^z\sigma_{j+k}^y)\sigma_{j+1}^z \cdots \sigma_{j+k-1}^z \quad \text{(C.3)}$$

The generating function $\Psi(\lambda, \mu, t)$ of the linear combination of these macrovariables, $\lambda\mathbf{X}_1 + \mu\mathbf{X}_2$, can be calculated exactly by diagonalizing $\lambda\mathbf{X}_1 + \mu\mathbf{X}_2$ in a well-known nonlinear transformation.[30] The results thus diagonalized are expressed in terms of fermion operators $\eta_q{}^+$, η_q as follows:

$$\lambda\mathbf{X}_1 + \mu\mathbf{X}_2 = \sum_{0\le q\le\pi} \omega_q(\eta_q{}^+\eta_q + \eta_{-q}^+\eta_{-q} - 1) \equiv \sum_{0\le q\le\pi} \omega_q\mathbf{X}_q \quad \text{(C.4)}$$

where $\omega_q = 2(\lambda + 2\mu \cos q)$.

$$\mathscr{H} = \sum_{0 \le q \le \pi} \mathscr{H}_q = \sum \{a_q(\eta_q^+ \eta_q + \eta_{-q}^+ \eta_{-q} - 1) - b_q(\eta_{-q}^+ \eta_q^+ + \text{h.c.})\}$$

$$a_q = \mu_B H + \sum_{k=1}^{m} (-1)^k (J_k^x + J_k^y) \cos kq \tag{C.5}$$

$$b_q = -\sum_{k=1}^{m} (-1)^k (J_k^x - J_k^y) \sin kq$$

$$\mathscr{H}^{(i)} = \sum_{0 \le q \le \pi} \mathscr{H}_q^{(i)}; \qquad \mathscr{H}_q^{(i)} = -\beta \mathscr{H}_q(\{J_x\} \to \{J_x^0\}, H \to H^0) \tag{C.6}$$

with the replacements $a_q \to a_q^0$ and $b_q \to b_q^0$.

Now the generating function $\Psi(\lambda, \mu, t)$ is defined by

$$\Psi(\lambda, \mu, t) = \text{Tr}[\exp(\lambda \mathbf{X}_1 + \mu \mathbf{X}_2) \exp(-it\mathscr{H}) \exp(\mathscr{H}^{(i)}) \exp(it\mathscr{H})]/\text{Tr} \exp \mathscr{H}^{(i)} \tag{C.7}$$

From the expressions (C.4)–(C.6), we obtain the following *extensive property*:

$$\Psi(\lambda, \mu, t) = C \exp[N\psi(\lambda, \mu, t)] \qquad \text{for large } N \tag{C.8}$$

where

$$\psi(\lambda, \mu, t) = \lim_{N \to \infty} N^{-1} \log \Psi = \frac{1}{2\pi} \int_0^{\pi} \log\{f(q, \lambda, \mu, t)(2 \cosh \epsilon_q^0)^{-2}\}\, dq \tag{C.9}$$

with $\epsilon_q^0 = [(a_q^0)^2 + (b_q^0)^2]^{1/2}$, and

$$f(q, \lambda, \mu, t) = \text{Tr}_{(q,-q)} \exp(it\mathscr{H}_q) \exp(\omega_q \mathbf{X}_q) \exp(-it\mathscr{H}_q) \exp \mathscr{H}_q^{(i)} \tag{C.10}$$

As in Appendix B, we introduce a new spin representation:

$$\begin{gathered} b_q^- = \eta_q \eta_{-q}, \qquad b_q^+ = \eta_{-q}^+ \eta_q^+, \qquad \eta_q \eta_{-q} + \eta_{-q}^+ \eta_q^+ = b_q^x \\ \eta_q^+ \eta_q + \eta_{-q}^+ \eta_{-q} = 2b_q^+ b_q^- = b_q^z + 1 \end{gathered} \tag{C.11}$$

Then it is sufficient to consider the subspace spanned by $|0, 0\rangle$ and $|-q, q\rangle = b_q^+|0, 0\rangle$ as in Appendix B. By the help of these considerations, the product of the matrices in (C.10) is calculated to take the form

$$\exp(it\mathscr{H}_q) \exp(\omega_q \mathbf{X}_q) \exp(-it\mathscr{H}_q) \exp(\mathscr{H}_q^{(i)}) = \begin{pmatrix} A_q' & B_q' \\ C_q' & D_q' \end{pmatrix} \tag{C.12}$$

Here, we have

$$\begin{aligned} A_q' &= (c_0 + s_0 c_2)\{e^{\omega_q}(c^2 + s^2 c_1^2) + e^{-\omega_q} s^2 s_1^2\} \\ &\quad - 2iss_0 s_1 s_2 (c + isc_1) \sinh \omega_q \\ D_q' &= (c_0 - s_0 c_2)\{e^{\omega_q} s^2 s_1^2 + e^{-\omega_q}(c^2 + s^2 c_1^2)\} \\ &\quad + 2iss_0 s_1 s_2 (c - isc_1) \sinh \omega_q \end{aligned} \tag{C.13}$$

where $\epsilon_q = (a_q^2 + b_q^2)^{1/2}$ and

$$\begin{aligned} c &= \cos(t\epsilon_q), & c_1 &= \cos\psi_q \equiv a_q/\epsilon_q \\ s &= \sin(t\epsilon_q), & s_1 &= \sin\psi_q, \\ c_2 &= \cos\psi_q^0 \equiv a_q^0/\epsilon_q^0, & c_0 &= \cos(t\epsilon_q^0) \\ s_2 &= \sin\psi_q^0, & s_0 &= \sin(t\epsilon_q^0) \end{aligned} \tag{C.14}$$

Therefore, $f(q, \lambda, \mu, t)$ is given by

$$\begin{aligned} f(q, \lambda, \mu, t) &= 2 + A_q' + D_q' \\ &= 2\{1 + \cosh\omega_q \cosh\epsilon_q^0 + (\sinh\omega_q \sinh\epsilon_q^0) \\ &\quad \times [\cos^2(t\epsilon_q)\cos\psi_q^0 + \sin^2(t\epsilon_q)\cos(2\psi_q - \psi_q^0)]\} \end{aligned} \tag{C.15}$$

From (C.8), the nonlinear relaxation of magnetization, for example, is given by

$$M(t) = M(0) + \frac{1}{\pi}\int_0^\pi \{\cos(2t\epsilon_q) - 1\} \tanh\left(\frac{1}{2}\epsilon_q^0\right) \sin\psi_q \sin(\psi_q - \psi_q^0)\, dq \tag{C.16}$$

This is an extension of a previous result.[31] It should be noted that

$$\lim_{t\to\infty} M(t) \neq M_{\text{eq}} \quad \text{(nonergodic)} \tag{C.17}$$

The nonlinear relaxation of the energy E and the variances of E and M can be immediately obtained from (C.8).

Now, we discuss the relation between the linear critical slowing down and nonlinear critical slowing down. In Ref. 31, we defined the nonlinear relaxation time $\tau_X^{(n,l)}$ of the macrovariable $\mathbf{X}$ by

$$\tau_X^{(n,l)} = \int_0^\infty \langle\mathbf{X}\rangle_t/\langle\mathbf{X}\rangle_0\, dt \propto (T - T_c)^{-\Delta^{(n,l)}} \tag{C.18}$$

while the linear relaxation time is defined[32,33] by

$$\tau_X^{(l)} = \int_0^\infty \langle\mathbf{X}(t)\mathbf{X}(0)\rangle_{\text{eq}}/\langle\mathbf{X}^2\rangle_{\text{eq}}\, dt \propto (T - T_c)^{-\Delta^{(l)}} \tag{C.19}$$

In Ref. 31, we asserted the following: (i) $\Delta^{(n,l)} \leqslant \Delta^{(l)}$; (ii) in general, $\Delta^{(n,l)} \neq \Delta^{(l)}$ in nonergodic systems, as shown near the critical field H_c at $T = 0$ in the linear XY model, in which $\Delta^{(n,l)} = \frac{1}{2}$ and $\Delta^{(l)} = 1$; and (iii) $\Delta^{(n,l)} = \Delta^{(l)}$ in ergodic systems. Quite recently, Rácz[35] discussed these problems on the basis of the dynamical scaling law.[36,37] According to his arguments, $\Delta^{(n,l)} = \Delta^{(l)} - \beta$, where β denotes the critical exponent of the order parameter $\mathbf{X}$ in equilibrium. Our results (i) and (ii) in Ref. 31 are consistent with the relation obtained by Rácz, but the conjecture (iii) holds only when $\beta = 0$.

Our conjecture (iii) has come from the simple argument that in ergodic systems the differences in the initial (or intermediate) stages of the relaxation are expected not to affect the divergence of the relaxation, and that anomalous (or critical) fluctuations will appear dominant in (or very close to) equilibrium, which will be attained by the final stage of the relaxation. In order to reconcile our arguments with the relation obtained by Rácz, we have to make the following modifications: The boundary between the nonlinear (initial or intermediate) stage and the linear (or final) stage becomes larger and larger as the system approaches the critical point T_c, and the deviation of the order parameter **X** from the equilibrium value at the boundary point may be proportional to $(T - T_c)^\beta$. Thus, the anomaly appearing in the final stage may be proportional to $(T - T_c)^\beta \tau^{(l)}$ from our definition of the nonlinear relaxation (C.18). Then, if we assume that the contribution from the nonlinear stage is no more divergent than $(T - T_c)^\beta \tau^{(l)}$, we obtain the relation $\Delta^{(n,l)} = \Delta^{(l)} - \beta$. This may be the simplest interpretation of the scaling derivation by Rácz.

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