Roundabout Relaxation: Collective Excitation Requires a Detour to Equilibrium

Hidetoshi Morita* and Kunihiko Kaneko

Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo, 3-8-1 Komaba, Meguro-ku, Tokyo 153-8902, Japan

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Relaxation to equilibrium after strong and collective excitation is studied by using a Hamiltonian dynamical system of a one-dimensional XY model. After an excitation of a domain of K elements, the excitation is concentrated to fewer elements, which are made farther away from equilibrium, and the excitation intensity increases logarithmically with K. Equilibrium is reached only after taking this roundabout route, with the time for relaxation diverging asymptotically as K^{γ} with $\gamma \approx 4.2$.

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Relaxation to equilibrium is one of the most important topics in nonequilibrium phenomena. The relaxation dynamics after weak excitation has been thoroughly investigated; it is represented as a superposition of the dynamics of excited modes, each of which depends on external parameters such as temperature. When several modes are strongly and collectively excited, on the other hand, interaction among the excited modes is not negligible, which may cause nontrivial dynamic behaviors that are not simply represented by the superposition of the excited modes. In particular, a set of the excited modes may form a partial system and give an internal state that cannot be determined solely with an external conditions. The relaxation will depend on the internal state, and, in turn, the internal state will dynamically change with the relaxation; such an interplay between the internal state and the relaxation is expected to be seen generally in systems far from equilibrium. We intend to search for some nontrivial and universal relaxation phenomena therein.

Previously the authors have reported such a novel relaxation phenomenon using a Hamiltonian dynamical system of the XY model with mean field (MF) coupling [1]; when a part of the system is highly excited, the relaxation progresses intermittently through bottlenecks by self-organizing a critical state for the partial excited system. Now it is interesting to study the relaxation in a corresponding lattice system. In particular we study a one-dimensional (1D) XY model, which has no phase transition and accordingly no critical state. In spite of its absence, we find a rather remarkable relaxation process, i.e., ''roundabout'' relaxation that a partially excited system reaches equilibrium only after it once goes farther away from equilibrium. In the present Letter, we report this discovery and analyze its mechanism by emphasizing the divergence of the relaxation time to equilibrium with the number of excited elements.

The Hamiltonian that we study is [2]

$$\mathcal{H} = \sum_{i=1}^{N} \left\{ \frac{p_i^2}{2} + J[1 - \cos(\theta_{i+1} - \theta_i)] \right\}, \qquad (1)$$

where $\theta_i \in [-\pi, \pi)$, with periodic boundary condition $\theta_i = \theta_{i+N}$. We consider the case of $J > 0$ (ferromagnetic), setting $J = 1$ without loss of generality. The N pendula, placed on the 1D lattice, are coupled by the nearest neighbor interaction. Each pendulum has two types of motion—rotation at a higher and libration at a lower energy.

Note that when a single element is highly excited, its relaxation is slow, with the relaxation time increasing exponentially with the excitation momentum, as in the case with MF coupling [3]. This is simply because the effective interaction between the excited element and the others rapidly decreases as the excitation momentum increases. The exponential dependence as such has been discussed in terms of the Boltzmann-Jeans conjecture (BJC) [4].

Here we study the relaxation when a domain of the system consisting of quite a few elements is highly excited, while the whole system is much larger [1]. To be specific, the system is prepared to be in equilibrium, with an energy density U and total momentum zero. At $t = 0$, K elements are simultaneously excited with the same momentum P_K. The momentum profile then becomes almost rectangular, with two domains separated by two interfaces. The number of the excited elements are much smaller than that of the total system, $K/N \ll 1$; we keep $K/N = 0.1$ in the following numerical simulation.

We first numerically observe the relaxation process. The element at the interfaces of the excited domain is intermittently absorbed into the nonexcited domain, losing its excited energy. The population of the excited elements $N^{(E)}$ accordingly decreases one by one from the initial K toward zero (equilibrium). If the excitation is strong enough, the excited domain receives some positive momentum from the escaped element, to increase its center-of-mass (c.m.) momentum; the process is repeated as the relaxation progresses (Fig. 1). The excited elements then rotate faster and faster, and thereby go farther away from equilibrium. The increase of the c.m. momentum implies more time for the next escape, as in the argument for BJC, and requires much longer time to reach equilibrium.

Thus the highly excited state is self-sustained, and the relaxation to equilibrium must take this roundabout route.

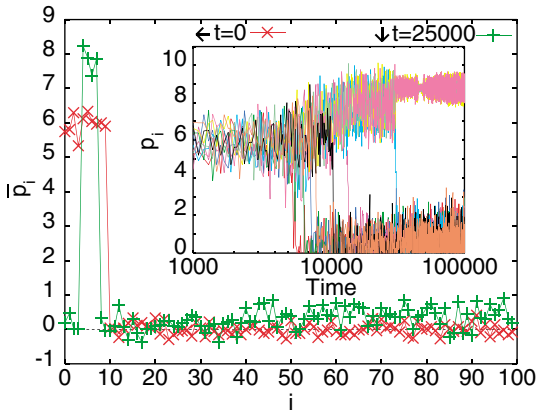

FIG. 1 (color). Two snapshots of the momentum profile $\overline{p}_i$, with $\bar{\cdot}$ as the time average over a period of 1000, at $t = 0$ and 25 000 (corresponding to the arrows to the inset). In the inset, the corresponding time series of the momenta of the excited elements are overlaid, where the abscissa axis is the logarithmic scale in time. $N = 100$, $K = 10$, $P_K = 6$, $U = 0.3$.

This process is not observed near equilibrium, and requires sufficient excitation of a domain of elements.

Here the system is composed of two domains through two interfaces. Since the momentum difference at the interface is very large, and the interaction decreases rapidly with it, the interaction across the interface is much weaker than that within each domain. In other words, the time scale of *interdomains* relaxation is much slower than that of *intradomain*, that is, equilibration within each domain. Then, from the inertial frame of each c.m. momentum, each domain is considered as almost in equilibrium at a first approximation. Hence the whole system is regarded as two thermodynamic systems weakly coupled through the interface.

Being large enough, the nonexcited system plays the role of a heat bath whose thermodynamic state is kept almost constant throughout the relaxation. The state of the excited domain, on the other hand, changes in the time scale much slower than *intradomain* equilibration time but much faster than the whole relaxation time to the equilibrium. Thus it is possible to define an *internal state* for the excited system as its thermodynamic state. To quantify the internal state, we introduce the *effective temperature* of the excited domain,

$$T^{(E)} \stackrel{\text{def}}{=} \frac{1}{N^{(E)}} \sum_i^{(E)} (p_i - P^{(E)})^2, \tag{2}$$

in the inertial frame with the following c.m. momentum of the excited domain,

$$P^{(E)} \stackrel{\text{def}}{=} \frac{1}{N^{(E)}} \sum_i^{(E)} p_i, \tag{3}$$

where $\sum^{(E)}$ denotes summation over only the excited elements.

To study the dynamics of the internal state, we calculate the change of the c.m. momentum, $\Delta P^{(E)}$, and of the effective temperature, $\Delta T^{(E)}$, of the excited domain, due to the first absorption of an interfacial element into the nonexcited (bath) part ($K \to K - 1$). Their dependence on $T_K \stackrel{\text{def}}{=} T^{(E)}|_{t=0}$ is plotted in Fig. 2, which is computed by preparing the excited state with T_K from a thermal equilibrium state with the c.m. momentum P_K. The figure shows that $\Delta T^{(E)}$ decreases toward 0 from the positive side, indicating that $T^{(E)}$ increases to approach a certain temperature. On the other hand, $\Delta P^{(E)}$ approaches a certain positive value. Except for the K dependence of the limit value of $\Delta P^{(E)}$, the other properties above are independent of any other parameter including U and sufficiently large P_K. By noting that single elements are absorbed successively in the relaxation course, the above result indicates that the effective temperature increases and approaches a high value, and there the c.m. momentum increases by some constant value per each absorption. The c.m. momentum of the excited domain thus continues to increase until the last element is absorbed while a high temperature at the excited domain is sustained.

Now we study the increase of the relaxation time with the number of the excited elements. Numerically it is not so easy to trace all the relaxation course, since it requires a huge time. Instead we give an analytical estimate for it by focusing on the dynamics of the macroscopic quantities of the excited part. To make notations simple in the following analysis, subscript $\cdot^{(E)}$ is omitted, and let $\cdot_m$ be macroscopic quantities when the number of the remaining excited elements is m.

First, we study how the change of the c.m. momentum $P_{m-1} - P_m$ depends on m. We numerically calculate $P_{K-1} - P_K$ with its dependence on K, which is plotted in Fig. 3. We have also confirmed numerically that the relationship is almost independent of the values of P_K or T_K, as long as they are large enough. Thus we obtain,

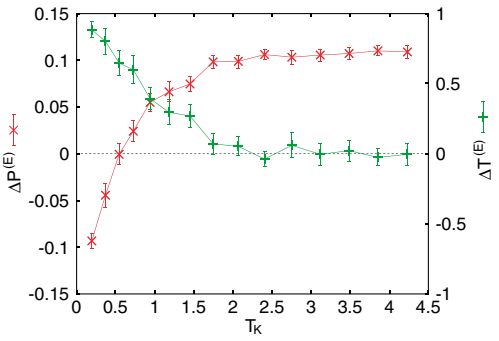

FIG. 2 (color). The change of the c.m. momentum, $\Delta P^{(E)}$ ($\times$, solid line), and the effective temperature, $\Delta T^{(E)}$ ($+$, dotted line), which are time averaged over a period of 100, against the (initial) effective temperature T_K. $N = 300$, $K = 30$, $P_K = 8$, $U = 0.3$. Obtained from the numerical calculations of 25 samples for each T_K.

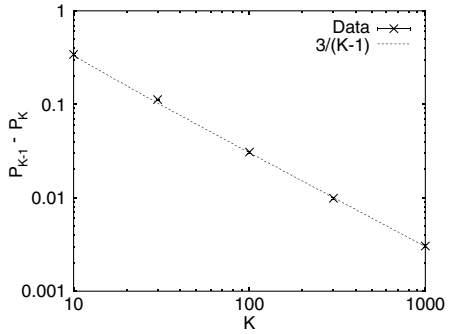

FIG. 3. $P_{K-1} - P_K$ vs K. Plotted for $P_K = 8$, $T_K \approx 2.4$, but this relationship is found almost independent of the values of P_K and T_K. Obtained from the numerical calculations of 100 samples for each K.

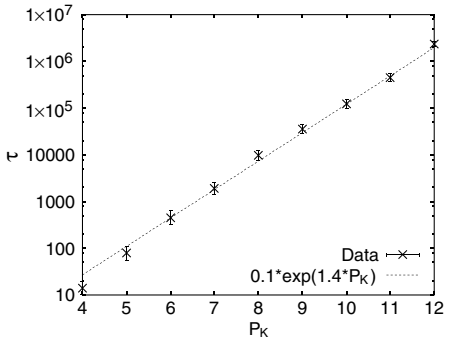

FIG. 4. τ versus P_K. $N = 300$, $K = 30$, $T_K \approx 2.4$. Obtained from the numerical calculations of 25 samples for each P_K.

for any $m \geq 2$,

$$P_{m-1} - P_m = \alpha/(m-1). \tag{4}$$

Here α is a constant with the dimension of momentum, which we numerically found $\alpha \approx 3$. We examine a rough estimation of the value by considering the dynamics of only three interfacial elements: an escaping element with two neighboring ones. Furthermore, the motion of each neighboring element is approximated as a constant rotation with the momentum 0 and Ω. Then the effective Hamiltonian of the interfacial dynamics can be given as

$$\mathcal{H}_{\text{inter}} = p^2/2 + J[1 - \cos\theta] + J[1 - \cos(\theta - \Omega t)]. \tag{5}$$

For $|\Omega| > \Omega_{\text{thr}} \approx 6$, two motions within the region around $p \sim 0$ and $p \sim \Omega$ are separated by KAM tori, while for $|\Omega| < \Omega_{\text{thr}}$, an orbit can cross between the two regions due to the collapse of the last KAM torus through the so-called "resonance overlap [5]." In other words, the interface element can jump over from $p \sim \Omega$ to $p \sim 0$ only if $|\Omega|$ is less than Ω_{thr}. Coming back to the original problem, this is nothing but the escape of the interfacial element from the excited domain. The loss of the momentum Ω_{thr} thereby should be compensated by the momentum gain of the neighboring elements, each of which is given approximately $\Omega_{\text{thr}}/2$ from the symmetry. Hence the excited domain gains momentum about $\Omega_{\text{thr}}/2$, which is distributed to the $m-1$ elements therein, leading to the increase of the c.m. momentum by $\Omega_{\text{thr}}/2/(m-1) \approx 3/(m-1)$.

Second, we compute the relaxation time τ when the first one of the excited elements loses its energy and is absorbed into the nonexcited part ($K \to K-1$), whose dependence on P_K is plotted in Fig. 4. This exponential dependence is just the form of the BJC mentioned above. This relationship again is almost not affected by K and T_K [6], as long as they are large enough. Thus we obtain

$$\tau(P) = Ce^{\beta P}. \tag{6}$$

The constant β has the dimension of inverse momentum, which is the order of the inverse of the momentum for the separatrix motion of a pendulum. Numerically we have obtained $\beta \approx 1.4$ and $C \approx 0.1$.

On the basis of the short-time properties (4) and (6), we estimate the long-term relaxation. First we consider the moment of the last excited element P_1. When the population falls to m from K, the gain of the c.m. momentum is

$$P_m - P_K = \sum_{j=m}^{K-1}(P_j - P_{j+1}) = \sum_{j=m}^{K-1}\frac{\alpha}{j} = \alpha(S_{K-1} - S_{m-1}), \tag{7}$$

by summing up (4), where $S_K \overset{\text{def}}{=} \sum_{j=1}^{K}(1/j)$, which increases asymptotically as $\log K$ with $K \to \infty$. The momentum of the last excited element P_1 is then

$$P_1 - P_K = \alpha S_{K-1} \to \log K. \tag{8}$$

Hence the c.m. momentum diverges asymptotically as $\log K$.

Finally, we estimate the total relaxation time to the equilibrium. From (6) and (7), the total time up to the relaxation from m to $m-1$ is given by

$$t_m = \sum_{j=m}^{K}\tau(P_j) = t_K e^{\gamma S_{K-1}}\sum_{j=m}^{K} e^{-\gamma S_{j-1}}, \tag{9}$$

where $\gamma \overset{\text{def}}{=} \alpha\beta$ is a dimensionless number. Then the relaxation time to equilibrium is estimated as

$$\tau_{\text{eq}} = t_1 = t_K e^{\gamma S_{K-1}}\left(1 + \sum_{m=1}^{K-1} e^{-\gamma S_m}\right). \tag{10}$$

Recalling $\log(m+1) < S_m \leq \log m + 1$ for $m \geq 1$, we get

$$e^{-\gamma} m^{-\gamma} \leq e^{-\gamma S_m} < (m+1)^{-\gamma}. \tag{11}$$

Combining (10) and (11) yields

$$1 + \sum_{m=1}^{K-1}\frac{e^{-\gamma}}{m^{\gamma}} \leq \frac{\tau_{eq}}{t_K} e^{-\gamma S_{K-1}} < 1 + \sum_{m=1}^{K-1}\frac{1}{(m+1)^{\gamma}}. \tag{12}$$

As $K \to \infty$, $e^{\gamma S_K} \to e^{\gamma \log K} = K^{\gamma}$, and

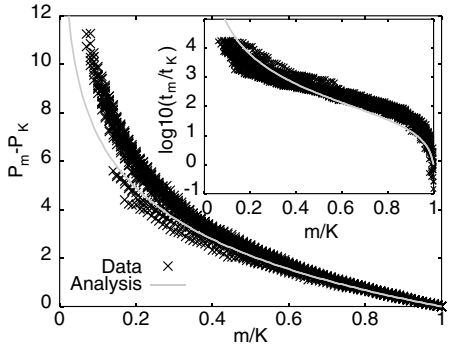

FIG. 5. Temporal change of P_m and t_m (inset), plotted against m/K, which decreases through the relaxation. Numerical results from 25 samples of direct relaxation simulations are plotted ($\times$), while the solid curves are the analytical estimation from (7) and (9), respectively. $N = 1000$, $K = 100$, $P_K = 8$, $T_K \approx 4.2$.

$$\sum_{m=1}^{K} \frac{1}{m^{\gamma}} \to \begin{cases} \zeta(\gamma) & \text{if } \gamma > 1 \\ \log K & \text{if } \gamma = 1 \\ K^{1-\gamma} & \text{if } 0 \le \gamma < 1, \end{cases} \tag{13}$$

where $\zeta(\cdot)$ is Riemann zeta. Hence the asymptotic form of the relaxation time to equilibrium τ_{eq} as $K \to \infty$ is

$$\tau_{\mathrm{eq}} \to \begin{cases} K^{\gamma} & \text{if } \gamma > 1 \\ K \log K & \text{if } \gamma = 1 \\ K & \text{if } 0 \le \gamma < 1. \end{cases} \tag{14}$$

Note that, if each excited elements relaxes independently, $\tau_{\mathrm{eq}} = K t_K$. Thus $\gamma = 1$ is the lower bound of the divergence attributed to the cooperative effect of the excited elements. Indeed, in the present model, we have $\alpha \approx 3$ and $\beta \approx 1.4$, and we get $\gamma \approx 4.2$. Hence the relaxation time satisfies $\tau_{\mathrm{eq}} \to K^{4.2}$, showing the rapid divergence with the number of excited elements. Since γ is dimensionless, this scaling is independent of J.

To check the validity of the above analysis, we have computed the increase of the c.m. momentum and the relaxation time up to the mth element, P_m and t_m (Fig. 5). Even though it is hard to follow all the relaxation courses numerically, the numerical results (crosses) plotted against m/K rather well agree with the theoretical estimates (7) and (9) (solid curves).

In summary, we have discovered that a class of one-dimensional lattice systems must take a ''roundabout relaxation route,'' once highly excited. After an excitation of a domain of the system, the momentum of the domain increases logarithmically to go farther away from equilibrium before reaching equilibrium. The relaxation time accordingly diverges as a power K^{γ} against the increase of the excited elements K. Hence the relaxation with collective excitation has a peculiar form, and is rather different from that near equilibrium.

The present result is expected to be general as long as the effective coupling of an excited part with the rest of the system decreases toward zero with the increase of the excitation intensity. First, we have carried out extensive numerical simulations for 2D, 3D, and 5D XY models by exciting a domain of elements. We have observed the present roundabout relaxation for all these models. At the same time, the excited domain tends to approach the critical point, as in the previous study with the MF model [1]. Thus both the self-organization of critical state (MF) and the increase of the excited momentum (1D) are observed in these intermediate dimensions. In physics there are several examples described as coupled pendula on a lattice, including Josephson junction arrays [7], or as a system satisfying the above decrease of effective coupling. Our result presents a novel scenario to slow relaxation therein.

Second, we have studied the present XY model with the addition of on-site sine potential, which is a nonintegrable variant of the sine-Gordon model that is known to show breather [8]. Here we have again observed the increase of c.m. momentum by absorbing the momenta of relaxing elements, leading to roundabout relaxation (see also [9]). Note that in the focusing phenomena [10,11], the energy of breathers increase by collision, to go farther away from equilibrium, up to some point. Possible relationships between the present roundabout relaxation and focusing in breather should be clarified in future.

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*Electronic address: morita@complex.c.u-tokyo.ac.jp

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