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Self-organized bottleneck in energy relaxation

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Abstract. – We study an energy relaxation process after many degrees of freedom are highly excited in a Hamiltonian system with a large number of degrees of freedom. Bottlenecks of relaxation, where relaxation of the excited elements drastically slows down, are discovered. By defining an internal state for the excited elements, it is shown that the drastic slowing-down occurs when the internal state is in a critical state. The relaxation dynamics brings the internal state into the critical state, and the critical bottleneck of relaxation is self-organized.

The relaxation process to equilibrium has gathered much attention of physicists over several decades. Although relaxation near equilibrium has been well formulated theoretically, the process far from equilibrium is not yet fully understood. When a system is excited weakly, it is described as a superposition of elementary excitations with weak interactions. When the excitation is strong, on the other hand, it is inevitable to take into account strong interactions of the excited modes, which may behave cooperatively. Even though a general theory for such case may not be available, it is important to find a class of novel relaxation phenomena, and propose novel physical concepts associated with it.

In this letter, we report a relaxation process when quite a few degrees of freedom are highly excited, in a simple Hamiltonian system with large degrees of freedom. The excited elements which interact strongly form a partial thermodynamic system, to which an internal state is assigned. The relaxation depends on this internal state, and, in turn, the internal state dynamically changes with the relaxation. We will show that, due to the interplay between the relaxation and the internal-state dynamics, the partial system self-organizes a critical state, which forms a bottleneck in the relaxation course.

As a specific model we adopt a Hamiltonian system [1, 2]:

$$H(\theta, p) = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{K}{2(2\pi)^2 N} \sum_{i=1}^N \sum_{j=1}^N [1 - \cos 2\pi(\theta_i - \theta_j)], \quad (1)$$

where K is set at 1, by properly scaling the units, without losing generality. The equations

of motion are given by

$$\frac{dp_i}{dt} = -\frac{K}{2\pi N} \sum_{j=1}^N \sin 2\pi(\theta_i - \theta_j), \quad (2)$$

where N pendula are globally coupled, interacting through phase difference. Each pendulum has two types of motion; rotation at a higher energy and libration at a lower energy.

In equilibrium, this system shows continuous phase transition in the thermodynamic limit $N \rightarrow \infty$ [2]. The order parameter M for this transition is the absolute value of the mean field, defined as $Me^{i2\pi\phi} = \sum_{j=1}^N e^{i2\pi\theta_j}/N$. When the total energy E is very small, $M \simeq 1$, where all the pendula librate. As the total energy increases, M decreases, where some pendula librate and others rotate, changing their types of motion temporally. Above a transition energy $E_c/N = 0.75/(2\pi)^2$ (corresponding transition temperature $T_c = 0.5/(2\pi)^2$), $M \simeq 1/\sqrt{N}$, and all the pendula rotate almost freely.

When a single element is excited, energy relaxation is very slow [3], with the relaxation time increasing as a stretched exponential form of the excited energy, as is discussed in terms of Boltzmann-Jeans conjecture [4, 5].

We are interested in relaxation properties when a part of the system composed of quite a few elements is excited, while the whole system is much larger. At $t = 0$, $N^{(k)}$ elements are simultaneously kicked, *i.e.* excited instantaneously, with the same momentum $P^{(k)}$. Instead of carrying out direct simulations of large- N system, we attach a heat bath with the temperature T to all the rest $N - N^{(k)}$ elements. In statistical mechanics, in general, it is expected that the system with this heat bath agrees with that of Hamiltonian dynamics as long as $N \gg N^{(k)}$. In the present case, with *global* coupling, this agreement may not be so evident. Hence we have also carried out direct simulations of Hamiltonian dynamics (without heat bath) for several values of temperatures, by taking a system with large N (say $N^{(k)} = 30$, and $N = 1000$). In fact the results to be presented (see, *e.g.*, the inset of fig. 3 below) are confirmed for all the temperature values we have examined. Instead of carrying out numerical simulations for such huge system for more temperature values and for more samples, we here present mainly the results obtained from the simulation of the above partial heat bath, but it should be remarked that the results here are also supported through simulations of full Hamiltonian dynamics. The equations of motion of the rest $N - N^{(k)}$ elements are given, instead of by (2), by the underdamped Langevin equation,

$$\frac{dp_i}{dt} = -\frac{K}{2\pi N} \sum_{j=1}^N \sin 2\pi(\theta_i - \theta_j) - \gamma p_i + \xi_i(t), \quad (3)$$

where $\xi_i(t)$ is white-Gaussian random noise, that is $\langle \xi_i(t) \rangle = 0$ and $\langle \xi_i(t_0)\xi_j(t_0 + t) \rangle = 2\gamma T \delta_{ij} \delta(t)$, with small γ ($\gamma = 0.01$ throughout the paper, while the result here is preserved as long as γ is small enough to satisfy underdamped regime).

A typical time series of the energy relaxation after the excitation is drawn in fig. 1. The excited elements, which rotate fast, relax one by one with losing their kinetic energy. The *population of excited elements* $N^{(E)}$ decrease from $N^{(k)}$ to zero, whose time series is drawn in fig. 2(a). It shows several plateaus, where the relaxation is drastically slowed down. We call these plateaus *bottlenecks* of the relaxation.

With regard to this intermittent appearance of the relaxation bottlenecks, we ask whether the bottlenecks appear all at random or follow some rule. If the latter is the case, the state of the excited partial system should be important, since the other huge part is kept at an almost constant temperature during the relaxation.

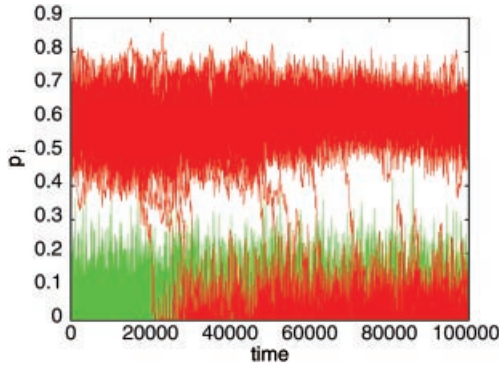


Fig. 1

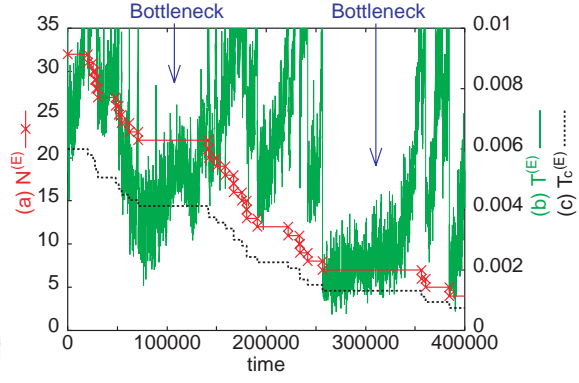


Fig. 2

Fig. 1 – A typical time series of momenta. $N = 64$, $T = 0.01$, $N^{(K)} = 32$, $P^{(K)} = 0.6$. The red ones are the initially excited elements, and the green ones are the rest.

Fig. 2 – A typical time series of (a) the population of excited elements $N^{(E)}$, (b) the effective temperature of the excited part $T^{(E)}$ (eq. (4)), and (c) the effective critical temperature $T_c^{(E)} = T_c N^{(E)} / N$ [6], which decreases along with $N^{(E)}$. The data are the same as in fig. 1.

Here, the interaction between the excited element and the non-excited one is small on the average, because the temporal average of the term $\sin 2\pi(\theta_i(t) - \theta_j(t))$ is negligible if the momenta of the two elements are much different. Indeed, this is the essence of long relaxation time scale in the Boltzmann-Jeans conjecture [3]. The interaction between two excited elements, on the other hand, can be strong, if the momenta are not much different. In fact, by taking a Galilean frame moving with the average velocity of the excited pendula, these two excited elements often librate each other, keeping attracting interactions.

Hence, our system is represented as two partial systems which are weakly coupled. One system is composed of excited elements whose momenta $\simeq P^{(E)}$, while the rest system has momenta $\simeq 0$. Since the interaction between the two partial systems are small, it is relevant to consider a thermodynamic state of each partial system at the first-order approximation, while the interaction with other elements is just a perturbation. Actually, temporally local thermodynamic quantities fulfill the equation of state in equilibrium, and the momentum distribution of each part roughly takes the form of a Maxwellian in our relatively small system, except for the time just before the relaxation of an element. Anyway, in this letter, we attempt to describe our phenomena only within such rough quantities [7].

The state of the relaxed part is basically determined by the heat bath with the temperature T . The state of the excited part, on the other hand, changes as the relaxation process progresses. Thus it is important to study a thermodynamic state of the excited part as an *internal state* of the whole system. As a quantity representing the internal state, we introduce the *effective temperature of the excited part* $T^{(E)}$ as

$$T^{(E)} = \frac{1}{N^{(E)}} \sum_i^{(E)} (p_i - P^{(E)})^2, \quad (4)$$

by taking an inertial frame with the center-of-mass momentum of the excited part $P^{(E)} = \sum_i^{(E)} p_i / N^{(E)}$, where $\sum^{(E)}$ denotes the summation over excited elements [8].

To see how the relaxation depends on the internal state, we define the *first relaxation time*

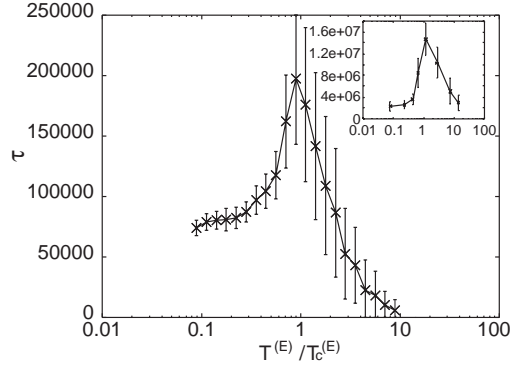


Fig. 3 – The first relaxation time τ vs. the effective temperature of the excited part $T^{(E)}$. $N = 32$, $T = 0.01$, $N^{(K)} = 16$, $P^{(K)} = 0.8$. 2000 samples are computed in all. $T^{(E)}$ is computed from the time average of (4) over a period of 1000 just after the elements are excited [9], while the time scale of microscopic motion is the order of 0.1 to 1. τ is averaged for the samples within the bin size of 0.1 for log scale. $T_c^{(E)}$ is the effective critical temperature. The inset is the corresponding one in the full Hamiltonian system. $N = 1000$, $E^{(R)} = 0.01$, $N^{(K)} = 30$, $N^{(K)} = 0.8$. 25 samples are averaged for each effective temperature, the value of which is, in this case, calculated from the total energy before attachment ($t < 0$).

τ as the time when the first one of $N^{(K)}$ elements loses its excited energy. In other words, τ is the first escape time of an element from the excited to the relaxed part. The relation between τ and $T^{(E)}$ is plotted in fig. 3. In order to control $T^{(E)}$, we adopt the following operation, instead of just kicking: we prepare two already equilibrated isolated systems, whose center-of-mass momenta are $P^{(K)}$ and 0, and then attach them at $t = 0$. Here, a peak is discernible. This is also true for a full Hamiltonian system (see the inset). Moreover, the temperature for this peak corresponds to the *critical* point for the phase transition of the excited part $T_c^{(E)} = T_c N^{(E)} / N$ [6], when the excited part is regarded as in equilibrium.

We have also computed the time series of $T^{(E)}$ (fig. 2(b)). The plateau of $N^{(E)}$ actually corresponds to the time when $T^{(E)}$ is around the critical temperature $T_c^{(E)}$ (fig. 2(c)). From these results it is concluded that the relaxation bottleneck occurs when the internal state is around a critical point.

Note that this phenomenon is different from a critical slowing-down of the excited part in two points. Firstly, the whole system is not in a critical state. In fact we verified that the coincidence of this peak position to the effective critical point is qualitatively independent of the heat bath temperature T . Secondly, such a peak is not found when disregarding the rest system. In fact we estimated the first escape time of an element in only a single isolated system, by calculating the time until one of the elements first takes a momentum smaller than a threshold. This escape time monotonically decreases as the temperature increases; it does not have any peak even at the critical point. Thus the present slow relaxation is *inter*-system relaxation, not *intra*-system relaxation to which the so-called critical slowing-down belongs.

Then how is the excited system stuck to the critical point through the interaction with the rest system? To answer this question, we consider how the internal state changes before and after one of the excited elements relaxes. To see this change, we introduce an *effective-temperature change* $\Delta T^{(E)}$ defined as

$$\Delta T^{(E)} = \frac{N^{(E)}}{N^{(E)} - 1} T_{\text{after}}^{(E)} - T_{\text{before}}^{(E)}, \quad (5)$$

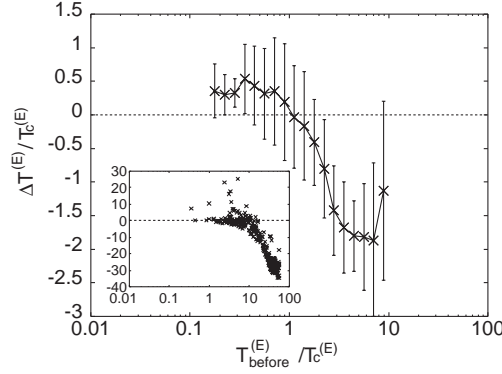


Fig. 4 – $\Delta T^{(E)}$ vs. $T_{\text{before}}^{(E)}$, computed from the simulations of fig. 3. The inset is the result from the full Hamiltonian dynamics (where the data for $T_{\text{before}}^{(E)} < T_c^{(E)}$ is very sparse, because such events are rare due to the increase of the temperature during the relaxation).

where $T_{\text{before}}^{(E)}$ and $T_{\text{after}}^{(E)}$ are the effective temperatures before and after the first relaxation of an excited element (τ), respectively, while the factor $N^{(E)}/(N^{(E)} - 1)$ comes from the contribution of scaling [6]. The relation between $\Delta T^{(E)}$ and $T_{\text{before}}^{(E)}$ is plotted in fig. 4. $T_{\text{before}}^{(E)}$ and $T_{\text{after}}^{(E)}$ are computed from the time average over a period of 1000 just before and after τ [9], respectively. The average of $\Delta T^{(E)}$ is positive when $T_{\text{before}}^{(E)} < T_c^{(E)}$, while it is negative when $T_{\text{before}}^{(E)} > T_c^{(E)}$. This result indicates that the internal state tends to be attracted into the critical state, through the interaction between the excited system and the rest.

To analyze the above effective-temperature dynamics, we note two factors [10]: the temperature increase of the excited part through the interaction with the relaxed part, and the temperature decrease through an escape of an element from the excited part.

Let us first consider the temperature increase of the excited part through the interaction with the relaxed part. The temperature change through this interaction is given by $\Delta T^{(E)} = \int dt \dot{T}^{(E)}(t)$ with

$$\dot{T}^{(E)} = \frac{2}{N^{(E)}} \sum_j^{(E)} p_j \dot{p}_j - 2P^{(E)} \dot{P}^{(E)}. \quad (6)$$

Using the order parameter of the partial systems $M^{(*)} e^{i2\pi\phi^{(*)}} = \sum_j^{(*)} e^{i2\pi\theta_j} / N^{(*)}$, where $*$ is E or R [8], we obtain the following expression, which is closed only in macroscopic variables:

$$\frac{d}{dt} E^{(E)} = \frac{N^{(R)}}{N} \frac{K}{(2\pi)^2} \{ \dot{M}^{(E)} + i2\pi(\dot{\phi}^{(E)} - P^{(E)}) M^{(E)} \} e^{i2\pi\phi^{(E)}} M^{(R)} e^{-i2\pi\phi^{(R)}}. \quad (7)$$

Here $E^{(E)}$ is the effective total energy of the excited part, given by

$$E^{(E)} = \frac{T^{(E)}}{2} + \frac{N^{(E)}}{N} \frac{K}{2(2\pi)^2} [1 - M^{(E)2}]. \quad (8)$$

$M^{(E)}$ relaxes in a potential field with some relaxation time scale [11]. The fluctuation of $\phi^{(E)} - P^{(E)}t$, on the other hand, does not have such time scale but is marginally stable, because it is the phase of the mean field of the excited part [12]. Thus, the first term of the r.h.s. of (7) can be neglected (adiabatically eliminated). With this approximation, the total energy

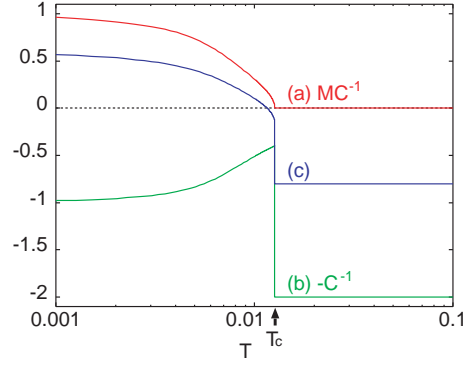


Fig. 5 – Temperature dependences of (a) MC^{-1} and (b) $-C^{-1}$ in the thermodynamic limit $N \rightarrow \infty$, which are obtained analytically by considering canonical distribution [2]. In the present mean-field model, the critical exponent of M at $T = T_c - 0$ is $1/2$. Hence the specific heat C does not diverge but takes a largest finite value. (c) is an example of combination of the two factors (a) and (b) with the ratio of $1 : 0.4$. The temperature of the horizontal axis is for a single system, and has to be scaled with $N^{(E)}/N$ to compare with fig. 4.

change $E^{(E)}$ of the excited part is proportional to $M^{(E)}$. Since $\Delta T^{(E)} \simeq \Delta E^{(E)}/C^{(E)}$, where $C^{(E)}$ is the effective specific heat of the excited part, we obtain

$$\Delta T^{(E)} \propto M^{(E)}/C^{(E)}. \quad (9)$$

Its temperature dependence in the thermodynamic limit of the excited part is calculated analytically by considering canonical distribution [2] (fig. 5(a)), which is positive at $T^{(E)} < T_c^{(E)}$ and vanishes for $T^{(E)} > T_c^{(E)}$.

Second, the temperature of the excited part decreases when an element escapes from the excited part, which has the largest negative momentum at the center-of-mass inertial frame of the excited part. This factor is estimated by calculating the decrease of temperature with the decrease of energy, by neglecting the interaction with the relaxed part. The escape of an element, with momentum p_{esc} measured from the center-of-mass inertial frame, takes away the energy $\Delta E_{\text{esc}} = p_{\text{esc}}^2/2$ from the excited part. Since temperature is a function of the total energy as $T^{(E)} = T^{(E)}(E^{(E)})$, the effective-temperature change eq. (5) can be described as $\Delta T^{(E)} = N^{(E)}/(N^{(E)} - 1)T^{(E)}(E^{(E)}) - T^{(E)}(E^{(E)} - \Delta E_{\text{esc}})$. In the limit $N^{(E)} \rightarrow \infty$, this is estimated by the specific heat $C^{(E)}$ as

$$\Delta T^{(E)} \simeq -\Delta E_{\text{esc}}/C^{(E)} \propto -1/C^{(E)}, \quad (10)$$

whose temperature dependence is drawn in fig. 5(b).

By combining above the factors, fig. 4 can be explained qualitatively (fig. 5(c)). $\Delta T^{(E)}$ is positive at a temperature below $T_c^{(E)}$. As the temperature approaches $T_c^{(E)}$ from below, $\Delta T^{(E)}$ decreases. Above $T_c^{(E)}$, there is only the negative contribution. Hence $\Delta T^{(E)}$ changes its sign from positive to negative as the temperature increases from below to above $T_c^{(E)}$.

In summary, by using a simple Hamiltonian system, we have discovered a bottleneck of energy relaxation, given by a critical state of an internal state of the excited part. This critical state is self-organized through the course of relaxation, once a *part* of a system is highly excited. The long-term relaxation from highly excited state to equilibrium consists of alternation between approach to critical state and collapse of the state. Although we

have demonstrated this bottleneck critical state by using a simple Hamiltonian system, the mechanism is expected to be general, as long as the system can exhibit continuous phase transition, and one part of the system is highly excited.

The self-organized bottleneck at a critical state may be observed in condensed matter, and in molecules with sufficiently large degrees of freedom, when a partial system is highly excited. The present bottleneck may shed new light on the understanding of such phenomena.

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REFERENCES

- [1] KONISHI T. and KANEKO K., *J. Phys. A*, **25** (1992) 6283.
- [2] ANTONI M. and RUFFO S., *Phys. Rev. E*, **52** (1995) 2361; YAMAGUCHI Y. Y., *Prog. Theor. Phys.*, **95** (1996) 717; CHOI M. Y. and CHOI J., *Phys. Rev. Lett.*, **83** (1999) 2104.
- [3] NAKAGAWA N. and KANEKO K., *J. Phys. Soc. Jpn.*, **69** (2000) 1255; *Phys. Rev. E*, **64** (2001) 055205(R).
- [4] BOLTZMANN L., *Nature*, **51** (1895) 413; JEANS J. H., *Philos. Mag.*, **6** (1903) 279; **10** (1905) 91; LANDAU L. D. and TELLER E., *Phys. Z. Sowjetunion*, **11** (1936) 18.
- [5] BENETTIN G., GALGANI L. and GIORGILLI A., *Commun. Math. Phys.*, **121** (1989) 557; BALDIN O. and BENETTIN G., *J. Stat. Phys.*, **62** (1991) 201.
- [6] The Hamiltonian (1) is scaled with K , by $(\theta, p, t, H) \rightarrow (\theta, \sqrt{K}p, t/\sqrt{K}, KH)$. Each element evolves by the equation of motion with factor K/N . Hence the excited part as a thermodynamic system is scaled with the effective coupling constant $K^{(E)}$ defined as $K/N = K^{(E)}/N^{(E)}$. Since the temperature is also scaled as $T \rightarrow KT$, the effective critical temperature $T_c^{(E)} = T_c K^{(E)}/K = T_c N^{(E)}/N$, which decreases as $N^{(E)}$ decreases.
- [7] Recently, the slow dynamics in this model is discussed in terms of Tsallis statistics, aging or glass dynamics; see, for example, LATORA V., RAPISARDA A. and RUFFO S., *Phys. Rev. Lett.*, **83** (1999) 2104; LATORA V., RAPISARDA A. and TSALLIS C., *Phys. Rev. E*, **64** (2001) 056134; MONTEMURRO M. A., TAMARIT F. A. and ANTENEODO C., *Phys. Rev. E*, **67** (2003) 031106; PLUCHINO A., LATORA V. and RAPISARDA A., cond-mat/0306374. So far our results here are understood without them, while it may be interesting to study the connection to them in future.
- [8] $\cdot^{(E)}$ and $\cdot^{(R)}$ stand for effective macroscopic quantities of the excited and the relaxed part, respectively, with the exception that $\sum^{(E)}$ and $\sum^{(R)}$ stand for summation over the elements of each part, respectively.
- [9] In case τ (or the second relaxation time τ_2) is smaller than 1000, the time average is calculated over τ (or τ_2), instead of 1000.
- [10] The same factors also seems to account for the coincidence of the peak with the critical point. We thank T. CHAWANYA, M. KIKUCHI, H. KENZAKI, and F. TAKAGI for discussion on this point.
- [11] LIFSHITZ E. M. and PITAEVSKII L. P., *Physical Kinetics* (Pergamon Press) 1981.
- [12] KURAMOTO Y., *Chemical Oscillations, Waves, and Turbulence* (Springer-Verlag) 1984.