Journal of Statistical Physics, Vol. 27, No. 2, 1982

Time Relaxation of the Solutions of Master Equations for Large Systems

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Received May 13, 1980; revised July 23, 1981

The time relaxation behavior of the solutions of certain classes of discrete master equations is studied in the limit of an infinite number of states. Depending on the range of the transition matrix, a relaxation behavior is found reaching from a $t^{-1/2}$ law for short range, over enhanced relaxation to an exponential relaxation for the extreme long-range case. The behavior in the limit of a continuous family of states is also discussed.

KEY WORDS: Time relaxation; master equations; diffusion; stochastic processes.

1. INTRODUCTION

It is a well-known fact that the solutions of the master equation with a finite number of states always show an exponential relaxation towards a stationary solution. Indeed, in the master equation

$$\dot{c}_n = \sum_{m=1}^{N} B_{nm} c_m, \qquad n = 1, \ldots, N \tag{1}$$

where

$$B_{nm} = A_{nm} - \delta_{nm} \sum_l A_{lm} \tag{2}$$

and

$$A_{nm} \geqslant 0, \qquad \forall n, m \tag{3}$$

the matrix B always has an eigenvalue zero, and the number of indepen-

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0022-4715/82/0200-0339$03.00/0

dent eigenvectors belonging to this eigenvalue is equal to its multiplicity. All other eigenvalues have strictly negative real parts, and since the total number of eigenvalues is finite the exponential relaxation of an arbitrary solution of (1) towards an equilibrium solution follows. For a discussion of these and some other quite general properties of the finite master equation, the reader is referred, e.g., to Refs. 1, 2.

Suppose now that we have a sequence of master equations with N increasing to infinity. Then for large N the real parts of the eigenvalues may accumulate and become dense at zero, and in the limit $N \to \infty$ this may drastically change the relaxation behavior. The conditions under which this happens, and the resulting relaxation behavior, will be discussed in this paper for a certain class of master equations. Assuming cyclic boundary conditions, the matrices (A_{ik}) will be supposed to be symmetric (microscopic reversibility) and translation invariant

$$A_{ik} = A_{ki} = A(i-k), \qquad \forall i, k \tag{4}$$

With these conditions, Eq. (1) can be interpreted as representing a continuous random walk problem on a one-dimensional lattice with periodic boundary conditions. The random walk on three-dimensional lattices is a frequently used model for the diffusion of atoms or defects in crystal lattices.[3] A part of our results extends trivially to the three-dimensional case.

If there are nearest neighbor transitions only, the general solution of (1), (4) for the infinite (one-dimensional) lattice is well known[4] and shows a relaxation towards the stationary solution (zero) following a $t^{-1/2}$ law. For the discrete time random walk on a lattice, the same kind of (discretisized) time relaxation has been shown to be true more generally if the second moments of the jump probabilities $\sum_k A_{ik}(k-i)^2$ are finite.[5] In Section 2 of this paper, the corresponding result for the continuous case is obtained. The condition $\sum_{r=1}^{\infty} A(r) r^2 < \infty$, $r = |i-k|$, is here called the condition of short range of $A(r)$. It is shown, if $A(r)$ is of short range, that the solutions $c_i(t)$ are approximated for large enough t by the function $\text{const} \cdot t^{-1/2}$ up to any desired degree of accuracy. This is shown by writing down the solution of the finite system and then considering the limit $N \to \infty$. For comparison, the explicit solution for $A(r) = \exp(-\alpha r)$, $\alpha > 0$, is briefly considered, and as a contrasting example the case where $A(r)$ is independent of r. In this latter case, the exponential relaxation is found to persist in the limit $N \to \infty$.

In Section 3 we investigate the time relaxation for an interesting class of matrices $A(r)$, which depend on r by a power law $A(r) \sim r^{-\alpha}$, $\alpha > 1$. Although for $\alpha > 3$ these $A(r)$ will be of short range, leading to a $t^{-1/2}$ relaxation, for $1 < \alpha \leqslant 3$ the short-range condition is not fulfilled and the relaxation behavior is changed for $N \to \infty$, now depending on α with the slowest term decaying as $t^{-1/(\alpha-1)}$. This is a faster relaxation than in the short-range cases. A qualitative change of behavior thus occurs at $\alpha = 3$, where also logarithmic functions are involved. The results of this section are also valid more generally if $A(r)$ has the form $A(r) = \text{const} \cdot r^{-\alpha} + A_1(r)$, where $r^{\alpha}A_1(r) \to 0$ for $r \to \infty$.

In Section 4 a further limit procedure is considered, now passing from a denumerable number of states to a continuum of states. The limit processes of the short-range type are then all related by a Wiener measure to random walks on continuous paths (and the system of differential equations can be shown to approach a diffusion equation). The limit process of the long-range example of Section 3 is similarly related by another measure, studied by P. Lévy,[6] to a random motion along discontinuous paths (the paths always incorporating sudden jumps). This result fits well to the observation in Section 3 of a quicker time relaxation in the countable long-range case. An attempt is made at verbally characterizing the dynamical difference between the various cases considered, which manifests itself in the relaxation behavior ranging from a $t^{-1/2}$ law over enhanced relaxation to an exponential type of relaxation.

In this paper, for simplicity we consider only systems with one-dimensionally ordered states. There is, however, no difficulty encountered in generalizing most of the results to multidimensional arrays. The relaxation behavior of the (translation invariant, symmetric) short-range cases is found to be like $t^{-d/2}$, where d is the dimensionality of the lattice of states.

2. THE FINITE SYSTEM AND THE INFINITE LIMIT OF SOLUTIONS. TIME RELAXATION IN THE SHORT-RANGE CASE

We start by writing down the general solution of the finite system (1) with the symmetry properties (4). Using the more convenient notation

$$\begin{aligned} A_{n,n+r} &= A_{n,n-r} =: A(r), && 0 \leqslant r < N/2 \\ A_{n,n+N/2} &=: 2A(N/2) && \text{if } N \text{ even} \end{aligned} \tag{5}$$

and letting $[x]$ be the largest integer less than or equal to x, we have

$$\dot{c}_n = \sum_{k=1}^{N} B_{nk} c_k = \sum_{r=1}^{[N/2]} A(r)(c_{n-r} + c_{n+r} - 2c_n), \qquad c_{n+N} = c_n \tag{6}$$

Equation (6) is immediately seen to have solutions of the type

$$c_n^k(t) = e^{-\omega_k t}\cos(2\pi kn/N) \qquad \text{and} \qquad c_n^{-k}(t) = e^{-\omega_k t}\sin(2\pi kn/N) \tag{7}$$

(and their linear combinations), where

$$\omega_k = -2 \sum_{r=1}^{[N/2]} A(r)\{\cos(2\pi kr/N) - 1\}, \qquad k = 0, 1, \ldots, [N/2] \quad (8)$$

Here we shall in particular be interested in the fundamental solutions, i.e., the solutions with the initial conditions $c_n(0) = \delta_{nm}$, m fixed. These are

$$c_{nm}(t) = \frac{1}{N}\epsilon_n + \frac{2}{N}\sum_{k=1}^{[N/2]} e^{-\omega_k t}\cos[2\pi(n-m)k/N], \qquad m \text{ fixed}, n = 1, \ldots, N \quad (9)$$

where

$$\epsilon_n = \begin{cases} 1, & N \text{ odd} \\ 1-(-1)^n, & N \text{ even} \end{cases} \quad (10)$$

The general solution is a linear combination of (9),

$$c_n(t) = \sum_{m=1}^{N} \lambda_m c_{nm}(t), \qquad n = 1, \ldots, N \quad (11)$$

with the initial conditions $c_n(0) = \lambda_n$.

Now let us examine what happens if N goes to infinity and let us denote by $c_{nm}^{(N)}$ the components of the solution (9) belonging to a given value of N. In order to obtain an integral in the limit, we introduce a new variable

$$\kappa = k/N \quad (12)$$

First we must study the behavior of ω_k, Eq. (8), when $N \to \infty$, $k \to \infty$, and $k/N \to \kappa$. Let us assume that $A(r)$ does not depend on N. Then

$$\omega_k \underset{\substack{N\to\infty \\ k/N\to\kappa}}{\longrightarrow} \omega_\kappa = -2\sum_{r=1}^{\infty} A(r)(\cos 2\pi\kappa r - 1) \quad (13)$$

$$= 4\sum_{r=1}^{\infty} A(r)\sin^2\pi\kappa r \quad (14)$$

the series converging uniformly if

$$\sum_{r=1}^{\infty} A(r) < \infty \quad (15)$$

With (15), ω_κ is continuous in κ and especially

$$\lim_{\kappa\to 0} \omega_\kappa = \omega_0 = 0 \quad (16)$$

If further

$$\sum_{r=1}^{\infty} A(r)r < \infty \tag{17}$$

then also the series

$$4\pi \sum_{r=1}^{\infty} A(r) r \sin 2\pi\kappa r \tag{18}$$

converges uniformly and can be integrated termwise. Hence (18) is the derivative of ω_κ and is continuous. Especially

$$\lim_{\kappa\to 0} \frac{d\omega_\kappa}{d\kappa}(\kappa) = \frac{d\omega_\kappa}{d\kappa}(0) = 0 \tag{19}$$

If $A(r)$ decreases faster still with increasing r, such that

$$\sum_{r=1}^{\infty} A(r) r^2 < \infty \tag{20}$$

then in the same way we see that the second derivative of ω_κ exists and is continuous, and thus at $\kappa = 0$

$$\lim_{\kappa\to 0} \frac{d^2\omega_\kappa}{d\kappa^2}(\kappa) = \frac{d^2\omega_\kappa}{d\kappa^2}(0) = 8\pi^2 \sum_{r=1}^{\infty} A(r) r^2 \tag{21}$$

which is strictly positive [except in the trivial case where all $A(r)$ are zero]. In this case we have

$$\omega_\kappa = \kappa^2 f(\kappa) \tag{22}$$

where $f(\kappa)$ is continuous and

$$f(\kappa) \underset{\kappa\to 0}{\longrightarrow} 4\pi^2 \sum_{r=1}^{\infty} A(r) r^2 > 0 \tag{23}$$

(This is most easily seen by applying de l'Hôpital's rule to ω_κ/κ^2.) For $\kappa > 0$, $f(\kappa)$ is twice continuously differentiable.

Having discussed ω_κ we may now turn to the equation (9), where we consider the same limit $N \to \infty$, $k \to \infty$, $k/N \to \kappa$. Let us be more definite about k:

$$k = [\kappa N] + 1 \tag{24}$$

i.e., k is the smallest integer larger than κN. Equation (9) obviously has the same limit as

$$\frac{1}{[N/2]} \sum_{k=1}^{[N/2]} e^{-\omega_k t} \cos[2\pi(n-m)k/N] \tag{25}$$

Under the assumption (15), however, the summands in (25) converge uniformly to a continuous function of κ, and therefore, for N large enough, (25) is arbitrarily close to an approximating sum to the Riemann integral of this continuous function, which again in the limit $N \to \infty$ (by definition) converges to the integral. Thus for the solutions with the initial conditions $c_{nm}^{(N)}(0) = \delta_{nm}$, m fixed, we have

$$\lim_{N\to\infty} c_{nm}^{(N)}(t) = c_{nm}(t) = 2\int_0^{1/2} d\kappa\, e^{-\omega_\kappa t}\cos 2\pi(n-m)\kappa \tag{26}$$

where ω_κ is given by (13). Let us remark that this result could also have been obtained by means of the Euler–Maclaurin summation formula[7] applied to (9), where the remainder term can be estimated to be of relative order $O(1/N)$.

$c_{nm}(t)$, Eq. (26), evidently goes to zero when t goes to infinity, but not necessarily in an exponential way as it does in the finite system. Most of the remainder of this paper will be concerned with the time dependence of $c_{nm}(t)$ under various assumptions on $A(r)$. In this section we examine the general case where $A(r)$ is of short range, i.e., such that (20) is valid, as well as an example of the extreme long range, where $A(r)$ does not at all depend on r (but is N dependent). In the following section we shall deal with an example of an intermediate range.

Let $A(r)$ be of short range. Then ω_κ is of the form (22) and, since (23) is different from zero, for small κ $f(\kappa)$ can be absorbed in a variable substitution

$$y = \kappa(f(\kappa))^{1/2} = (\omega_\kappa)^{1/2} \tag{27}$$

with

$$\frac{dy}{d\kappa} = \frac{1}{2(\omega_\kappa)^{1/2}}\,\frac{d\omega_\kappa}{d\kappa} \underset{\kappa\to 0}{\longrightarrow} \left[\frac{1}{2}\,\frac{d^2\omega_\kappa}{d\kappa^2}(0)\right]^{1/2} > 0 \tag{28}$$

where $dy/d\kappa$ is continuous and the limit follows by de l'Hôpital's rule [on $(dy/d\kappa)^2$]. Thus (27) can be inverted in a neighborhood of $\kappa = 0$, and for y_0 in this neighborhood

$$c_{nm}(t) = 2\int_0^{y_0} dy\,\frac{d\kappa}{dy}(y)e^{-y^2 t}\cos[2\pi(n-m)\kappa(y)] + 2\int_{\kappa(y_0)}^{1/2} d\kappa\, e^{-\omega_\kappa t}\cos 2\pi(n-m)\kappa \tag{29}$$

For small enough y_0, the nonexponential part of the first integrand can be replaced by its value at $y = 0$, thereby introducing an error less than an $\epsilon > 0$, which can be chosen arbitrarily small. A subsequent shift of the upper limit of integration to infinity introduces an exponentially decaying correction term. The second integral is also exponentially decaying. Noting that

$$\int_0^\infty dy\, e^{-y^2 t} = \frac{1}{2}\pi t^{-1/2} \tag{30}$$

we therefore obtain

$$c_{nm}(t) = at^{-1/2} + r(t) \tag{31}$$

where

$$a = \pi^{1/2}\left[\frac{1}{2}\frac{d^2\omega_\kappa}{d\kappa^2}(0)\right]^{-1/2} = \frac{1}{2}\left[\pi\sum_{r=1}^{\infty} A(r) r^2\right]^{-1/2} \tag{32}$$

and

$$|r(t)| < \epsilon\pi^{1/2} t^{-1/2} + at^{-1/2} e^{-y_0^2 t} + e^{-\omega' t} \tag{33}$$

with

$$\omega' = \min_{\kappa(y_0) \leqslant \kappa \leqslant 1/2} \omega_\kappa \tag{34}$$

In view of (14), ω' is positive.

For large t, $c_{nm}(t)$ thus deviates from the function $at^{-1/2}$ by a relative error less than $\epsilon\pi^{1/2}/a$, where ϵ can be chosen arbitrarily small.

The same can be shown for the $N \to \infty$ limit of the general solution (11), if the initial conditions $\{c_m^{(N)}(0)\}$ converge uniformly to $\{c_m(0)\}$ with $\sum_m c_m(0) < \infty$. Then

$$c_n^{(N)}(t) \underset{N\to\infty}{\longrightarrow} c_n(t) = 2\int_0^{1/2} d\kappa\, e^{-\omega_\kappa t} g_n(\kappa) \tag{35}$$

where $g_n(\kappa)$ is the continuous sum of the uniformly in κ convergent series $\sum_m c_m(0)\cos 2\pi\kappa(n-m)$, n fixed, and by exactly the same way of reasoning as above, the asymptotic behavior of $c_n(t)$ is $\sim t^{-1/2}$, if $A(r)$ is of short range [i.e., if (24) is valid]. It was already mentioned that this generalizes to $t^{-d/2}$ for $A(r_1, \ldots, r_d)$ describing symmetric, translation-invariant transition probabilities in a d-dimensional array of states.

As an explicit example of the short-range behavior, let us very briefly consider the master equation with an exponentially decreasing transition probability

$$A(r) = e^{-\alpha r}, \qquad \alpha > 0 \tag{36}$$

From (13) one obtains

$$\omega_\kappa = \frac{\gamma\beta\sin^2\pi\kappa}{1 + \beta\sin^2\pi\kappa} \tag{37}$$

where

$$\gamma = \coth\alpha, \qquad \beta = e^{-\alpha}/\sinh^2\alpha \tag{38}$$

As expected, ω_κ has the form (22). Now

$$\frac{\gamma\beta\sin^2\pi\kappa}{1+\beta} \leqslant \omega_\kappa \leqslant \gamma\beta\sin^2\pi\kappa \tag{39}$$

and hence from (26)

$$e^{-\gamma\beta t/2} I_{n-m}\left(\tfrac{1}{2}\gamma\beta t\right) \leqslant c_{nm}(t) \leqslant \exp\left(-\frac{1}{2}\,\frac{\gamma\beta t}{1+\beta}\right) I_{n-m}\left(\frac{1}{2}\,\frac{\gamma\beta t}{1+\beta}\right) \tag{40}$$

where $I_n(z)$ is the nth-order modified Bessel function [7]. For large t, therefore, both sides behave as[7] const $\cdot\, t^{-1/2}$. Comparison with (31), (32) shows that the lower limit is the best possible, since

$$\epsilon^{-\beta\gamma t/2} I_n\left(\tfrac{1}{2}\gamma\beta t\right) \sim (\pi\gamma\beta t)^{-1/2} \qquad \text{for } t \text{ large} \tag{41}$$

Let us now discuss an example, which in some sense is an extreme opposite of the above case, namely, where $A(r)$ does not at all depend on r. We shall have $A(r)$ depend on N though, and therefore some remarks are in order: (i) The uniform convergence and continuity implications of (15), (17), and (20), which were used above, do not follow generally without conditions on the convergence in N of $A^{(N)}(r)$ to $A^{(\infty)}(r)$. A sufficient supplementary condition to ensure the continuity of the kth derivative is $N[A^{(N)}(r) - A^{(\infty)}(r)]r^k \to 0$, if $N \to \infty$, uniformly for $r = 1, \ldots, N$. (ii) If, however, ω_κ [Eq. (13)] is continuous at $\kappa = 0$, it is easily deduced from Eq. (26) that the time relaxation is slower than any exponential term $e^{-\omega' t}$. This is not the case in the example that now follows. Let

$$A_{ik}^{(N)} = \frac{1}{N}, \qquad \forall i, k \tag{42}$$

Then (15) is valid, but (8) fails to have a continuous limit. Indeed, Eqs. (8), (5) render $\omega_k = 1 - \delta_{k0}$, and therefore the infinite limit ω_κ has a discontinuity at $\kappa = 0$,

$$\omega_\kappa = \begin{cases} 1, & \kappa \neq 0 \\ 0, & \kappa = 0 \end{cases} \tag{43}$$

The limit of (9) can be calculated as before, and (26) becomes

$$\lim_{N\to\infty} c_{nm}^{(N)}(t) = e^{-t} 2\int_0^{1/2} d\kappa \cos 2\pi\kappa(n-m) = e^{-t}\delta_{nm} \tag{44}$$

showing an exponential decay of the initial state also in the infinite limit.

Finally, let us remark that instead of solving the finite system of equations and considering the limit of the solutions as the number of states N goes to infinity, we could have started out from the infinite system of differential equations in the beginning [assuming (15)]. The question of uniqueness of the solutions is here a nontrivial one,[8,9] but if the initial conditions satisfy $\sum_n c_n(0) < \infty$, there is a unique solution that is Fréchet-differentiable as an element of l^1, as Banach space of sequences $\{x_n\}_{n=-\infty}^{\infty}$ with the norm $\sum_n |x_n| < \infty$.[9] It can be shown that the solutions of the finite systems considered above, when N goes to infinity, converge in the l^1-norm precisely to this Fréchet-differentiable solution of the infinite system.

3. A LONG-RANGE EXAMPLE

We now come to an interesting example, where the enhanced time relaxation in the case of a long-range transition matrix A is observed. In this model (which will be generalized at the end of the section), A_{ik} depends on $|i-k|$ according to a power law

$$A_{ik} = A(r) = r^{-\alpha}, \qquad r = |i-k|, \qquad \alpha > 1 \tag{45}$$

where α is taken to be larger than one in order to ensure that (15) exists. For $\alpha > 3$, A is of short range according to (20) and therefore the relaxation of $c_n(t)$, Eq. (26), is by a $t^{-1/2}$ law. For smaller α, however, (20) no longer holds and the relaxation behavior is different.

Inserting (45) in (13) we have

$$\omega_\kappa = -2 \sum_{r=1}^{\infty} \frac{1}{r^\alpha} (\cos 2\pi\kappa r - 1) \tag{46}$$

which can be naturally expressed by the function $\phi(z, \alpha)$,

$$\phi(z, \alpha) = \sum_{r=1}^{\infty} \frac{z^r}{r^\alpha}, \qquad |z| \leqslant 1 \tag{47}$$

which is a generalization of Riemann's zeta function

$$\zeta(\alpha) = \sum_{r=1}^{\infty} r^{-\alpha} = \phi(1, \alpha)$$

We have

$$\omega_\kappa = 2\phi(1, \alpha) - \phi(e^{2\pi i\kappa}, \alpha) - \phi(e^{-2\pi i\kappa}, \alpha) \tag{48}$$

The analytic continuation of $\phi(z, \alpha)$, Eq. (47), has been studied by E. Lindelöv,[10] who found an expansion in terms of $\log z$ at the point $z = 1$,

$\phi(1,\alpha) = \zeta(\alpha)$, valid for $|\log z| < 2\pi$:

$$\phi(z,\alpha) = \Gamma(1-\alpha)(-\log z)^{\alpha-1} + \sum_{r=0}^{\infty} \zeta(\alpha - r)\frac{(\log z)^r}{r!} \tag{49}$$

if $\alpha \neq 1,2,3,\ldots,$ and if $\alpha = 2,3,\ldots,$

$$\phi(z,\alpha) = \sum_{r=0}^{\infty}{}' \zeta(\alpha - r)\frac{(\log z)^r}{r!} + \frac{(\log z)^{\alpha-1}}{(\alpha-1)!}\left[\sum_{k=1}^{\alpha-1}\frac{1}{k} - \log\left(\log\frac{1}{k}\right)\right] \tag{50}$$

where the term $r = \alpha - 1$ is to be omitted in the first sum.

In (48) $\log z = \pm i2\pi\kappa$ with $0 \leqslant \kappa \leqslant 1/2$, and thus (49), (50) can be used. Collecting terms, we have

$$\omega_\kappa = -2\Gamma(1-\alpha)\cos\left[\frac{(\alpha-1)\pi}{2}\right](2\pi\kappa)^{\alpha-1} + 2\sum_{r=1}^{\infty}\zeta(\alpha-2r)(-1)^{r-1}\frac{(2\pi\kappa)^{2r}}{(2r)!} \tag{51}$$

for $\alpha \neq 1,3,5,\ldots,$ and

$$\omega_\kappa = \frac{(-1)^{(\alpha+1)/2}}{(\alpha-1)!}\left[\sum_{k=1}^{\alpha-1}\frac{1}{k} - \log(2\pi\kappa)\right](2\pi\kappa)^{\alpha-1} + 2\sum_{\substack{r=1\\ 2r\neq\alpha-1}}^{\infty}{}' \zeta(\alpha-2r)(-1)^{r-1}\frac{(2\pi\kappa)^{2r}}{(2r)!} \tag{52}$$

if $\alpha = 3,5,\ldots$. For an even integer α, ω_κ is a polynomial, since $\zeta(-2n) = 0$, $n = 1,2,\ldots$. For all other values of α, ω_κ is nonanalytical at $\kappa = 0$. If $\alpha > 3$, which is the short-range case, the lowest-order term in (51) and (52) is proportional to κ^2 and thus ω_κ is of the form (22) as it should be. For $\alpha < 3$, however, the lowest-order term is proportional to $\kappa^{\alpha-1}$, which now determines the time relaxation behavior of $c_n(t)$. For $\alpha = 3$ a logarithm appears in the lowest-order term, const $\cdot\, \kappa^2 \log\kappa$.

Consider the case $\alpha < 3$. ω_κ is of the form

$$\omega_\kappa = a\kappa^{\alpha-1} + \kappa^2 F(\kappa) \tag{53}$$

where $F(\kappa)$ is a power series in κ^2, and $F(0) \neq 0$. Therefore

$$\kappa^{-(\alpha-1)}\omega_\kappa \underset{\kappa\to 0}{\longrightarrow} a = (2\pi)^{\alpha-1}\left[-2\Gamma(1-\alpha)\cos\tfrac{1}{2}\pi(\alpha-1)\right] \tag{54}$$

and

$$\kappa^{-(\alpha-2)}\frac{d\omega_\kappa}{d\kappa}(\kappa) \underset{\kappa\to 0}{\longrightarrow} (\alpha-1)a \tag{55}$$

Now let

$$y = (\omega_\kappa)^{1/(\alpha-1)} \tag{56}$$

Then

$$\frac{dy}{d\kappa} = (\omega_\kappa)^{-(\alpha-2)/(\alpha-1)} \frac{d\omega_\kappa}{d\kappa} \underset{\kappa\to 0}{\longrightarrow} (\alpha-1)a^{1/(\alpha-1)} \neq 0 \tag{57}$$

and we can proceed exactly as in Section 2 for the short-range case, to find

$$c_n(t) = \frac{2}{\alpha-1} a^{-1/(\alpha-1)} \int_0^\infty dy\, e^{-y^{\alpha-1}t} + r(t) \tag{58}$$

with

$$|r(t)| < \frac{2}{\alpha-1} a^{-1/(\alpha-1)} \int_{y_0}^\infty dy\, e^{-y^{\alpha-1}t} + 2\epsilon \int_0^\infty dy\, e^{-y^{\alpha-1}t} + 2\int_{\kappa(y_0)}^{1/2} d\kappa\, e^{-\omega_\kappa t} \tag{59}$$

where y_0 is chosen such that

$$\left|\cos\left[2\pi\kappa(y)\right] \frac{d\kappa}{dy} - (\alpha-1)^{-1} a^{-1/(\alpha-1)}\right| < \epsilon \tag{60}$$

for all $y < y_0$, given an arbitrary $\epsilon > 0$. Further

$$\int_0^\infty dy\, e^{-y^{\alpha-1}t} = t^{-1/(\alpha-1)} \Gamma\left(\frac{\alpha}{\alpha-1}\right) \tag{61}$$

and we obtain

$$c_n(t) = bt^{-1/(\alpha-1)} + r(t) \tag{62}$$

with

$$b = \frac{2}{\pi(\alpha-1)} \Gamma\left(\frac{\alpha}{\alpha-1}\right)\left[-2\Gamma(1-\alpha)\cos\frac{1}{2}\pi(\alpha-1)\right]^{-1/(\alpha-1)} \tag{63}$$

and

$$|r(t)| < 2\epsilon\Gamma\left(\frac{\alpha}{\alpha-1}\right)t^{-1/(\alpha-1)} + e^{-y_0^{\alpha-1}t} d(t) \tag{64}$$

where

$$d(t) = 1 + b2^{(2-\alpha)/(\alpha-1)}\left[t^{-1/(\alpha-1)} + y_0^{2-\alpha}\Gamma\left(\frac{1}{\alpha-1}\right)^{-1} t^{-1}\right] \tag{65}$$

In contrast to the short-range case, while we still have a power law, the time relaxation exponent now depends on α. The sudden change in the α dependence occurs at the value $\alpha = 3$, which shows an intermediary behavior deriving from the presence of a logarithm in the lowest-order term of

(52). Indeed, if $\alpha = 3$, we can show that for any $\beta > 0$ and any positive constants c_1 and c_2, there exists a t_0 such that for $t > t_0$

$$c_1 t^{-1/(2-\beta)} < c_n(t) < c_2 t^{-1/2} \tag{66}$$

The above results are also valid in the more general case where $A(r)$ is of the form

$$A(r) = \text{const} \cdot r^{-\alpha} + A_1(r) \tag{67}$$

with

$$r^\alpha A_1(r) \underset{r\to 0}{\longrightarrow} 0 \tag{68}$$

since the addition of $A_1(r)$ will not affect the lowest-order term in ω_κ. And as in the short-range case, the results also extend to solutions $c_n(t)$ with arbitrary initial conditions $c_n(0)$ satisfying $\sum_n c_n(0) < \infty$.

4. THE CONTINUUM LIMIT. PATH INTEGRALS AND ORDERING

In the preceding sections we studied the time relaxation obtained in the limit of large systems governed by a discrete master equation. We observed a fundamental difference in the relaxation behavior according to whether the second moment of $A(r)$ existed or not. If it existed, the relaxation behavior was universally like $t^{-1/2}$, otherwise it was quicker and depended on the form of $A(r)$ more sensitively.

The fundamental difference between the short-range and long-range cases is again very clearly seen if the continuum limit is taken. Interpret n as numbering the points of a one-dimensional lattice with a lattice constant h (e.g., think of the problem of particle diffusion in a crystal). Write $x = hn$ and let h go to zero, keeping x fixed. This continuum limit corresponds to changing the scale on which observation is made completely towards the macroscopic regime. A change in the time scale is also necessary in order that the relaxation can be observed at finite times.

Let $A(r)$ be of short range and consider the general solution of (49), with (26),

$$c_n(t) = \sum_{m=-\infty}^{\infty} 2\int_0^{1/2} d\kappa\, e^{-\omega_\kappa t} \cos[2\pi(n-m)\kappa] c_m(0) \tag{69}$$

Let the initial values be given as

$$c_m(0) = v(hm), \qquad \text{where } \int_{-\infty}^{\infty} dy\, v(y) < \infty \tag{70}$$

Denote $x = hn$, $y = hm$, $\tau = t/h^2$, and $k = \kappa/h$, and let $h \to 0$, keeping x

and τ fixed. Then

$$c_n(t) \underset{\substack{h\to 0\\ hn\to x\\ t/h^2\to\tau}}{\longrightarrow} u(x,\tau) = 2\int_{-\infty}^{\infty} dy \int_0^{\infty} dk\, e^{-ak^2\tau}\cos[2\pi k(x-y)]v(y)$$

$$= \left(\frac{\pi}{at}\right)^{1/2}\int_{-\infty}^{\infty} dy\, e^{-\pi^2(x-y)^2/at}v(y) \tag{71}$$

where $a = 4\pi^2\sum_{r=1}^{\infty}A(r)r^2$. This is a solution of the one-dimensional diffusion equation

$$\begin{aligned} \partial_\tau u(x,\tau) &= \kappa_0\partial_{xx}u(x,\tau)\\ u(x,\tau=0) &= v(x) \end{aligned} \tag{72}$$

with the diffusion constant $\kappa_0 = \sum_{r=1}^{\infty}A(r)r^2$. Equation (72) can also be obtained directly as the continuum limit of the master equation itself, if and only if $\sum_{r=1}^{\infty}A(r)r^2 < \infty$. The solution Eq. (71) behaves as $t^{-1/2}$ for large t, and since the continuum limit involved only a scale transformation of the time, it again follows that the short-range processes all must have the same relaxation behavior. This is not so for the long-range processes of Section 4. With the same notation as above, but with the time scaling $\tau = t/h^{\alpha-1}$, we obtain

$$c_n(t) \underset{\substack{h\to 0\\ hn\to x\\ t/h^{\alpha-1}\to\tau}}{\longrightarrow} u(x,\tau) = 2\int_{-\infty}^{\infty} dy \int_0^{\infty} dk\, e^{-bk^{\alpha-1}t}\cos[2\pi k(x-y)]v(y) \tag{73}$$

where $b = -2\Gamma(1-\alpha)\cos\frac{1}{2}\pi(\alpha-1)$, and this is not a solution of a diffusion equation. It satisfies the differential–integral equation

$$\partial_\tau u(x,\tau) = P\int_{-\infty}^{\infty} dy\, \frac{1}{|y|^\alpha}\left[u(x+y)-u(x)\right] \qquad (P = \text{principal value}) \tag{74}$$

which can be obtained by applying the same limit procedure to the master equation itself, provided $1 < \alpha < 3$. The form of the integration kernel is that of $A(r)$ itself, so here the details of $A(r)$ are clearly more important than in the short-range cases, where only the second moment of $A(r)$ remained in the equations after the continuum limit was taken. In particular, the relaxation behavior here depends explicitly on α.

We finish with some rather speculative remarks on dynamical ordering. Let c_n be the probability of occupation of a state (or site) n. The states are of course ordered by their numbers, but this numbering is in principle arbitrary. However, a certain dynamical order of states (or "topology" of states) is established if $A(r)$ becomes smaller as r increases. If $A(r)$ is monotonous this ordering is strict. Let us illustrate this point by considering two extreme cases. If there are nearest neighbor transitions only, a state j can be reached from a state i only by going through all intermediate states and thus there is dynamically a strict order present, which coincides with the number order. If on the other hand $A(r)$ is independent of r, then from a dynamical viewpoint all states are equally close to the initial state and thus there is no dynamical ordering. In Section 2 we saw that in the former case the relaxation to the equilibrium solution obeyed a $t^{-1/2}$ law, whereas in the latter case we found an exponential relaxation. We also saw that the $t^{-1/2}$ law was valid for all $A(r)$ that diminished fast enough with r to satisfy the condition (24), which we called the condition of short range. It is now tempting to speculate that the short-range cases all describe processes, which in some sense are essentially local relative to the dynamical ordering of the states, and that for the long-range cases the different relaxation is perhaps a measure of the deviation from this locality. For the continuum limit this can be made more concrete. Consider $u(x,t)$, Eqs. (71), (73), and define by a function $x(t)$ a path through the states x. Then the kernel of (71) has an interpretation as (the density of) the Wiener measure[11, 12] of the continuous paths connecting x and y such that $x(0) \in (y, y + dy)$ and $x(t) = x$. The kernel (73) of the long-range case, on the other hand, turns out to be a measure not on the continuous paths only, but rather on the collection of left (or right) continuous paths with discontinuities of the first kind (finite jumps), whereby the continuous paths have zero measure.[12, 6] In the continuum limit, we are thus led to the interpretation that the short-range cases describe processes where the change is local in the sense of continuous paths (or evolution of a sample), whereas in the long-range cases, while the (dynamical) ordering may still be there, it is partly overruled by the change being not entirely local but always also including jumps over some distance. The continuous path cases have a $t^{-1/2}$ type of relaxation, whereas for the discontinuous path cases we obtain a quicker relaxation, $\sim t^{-1/(\alpha-1)}$, $1 < \alpha < 3$. Finally, the continuum limit of the extreme long-range case of section 2, Eq. (44), which has no (finite) path ordering, still has an exponential relaxation.

ACKNOWLEDGMENTS

The author would like to thank Professor A. Thellung for valuable discussions and a critical reading of the manuscript. He also acknowledges financial support from the Schweizerischer Nationalfonds.

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