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Transition behaviour in the asymptotic long-time limit and theoretical approach

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Abstract

To explore the two different long-time limit behaviours (decaying and non-decaying to zero for $t \to \infty$) of a dynamical quantity, we present a theoretical approach which analyses a continued fraction (CF) representation of the quantity. On the basis of our analysis, we show that the two asymptotic behaviours are characterized by a structure of CF coefficients, and that there exists a certain condition that determines the transition between the two limits. In addition a measure is introduced to predict the transition. We apply our theory to various systems to confirm its validity. The nondecay behaviour involves a kind of feedback process in a dynamical system. The appearance of a dynamical similarity near the transition is discussed.

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1. Introduction

Understanding the asymptotic long-time t (or small-frequency ω) behaviour for a dynamical quantity of interest, say a function $F(t)$, is one of the important problems in dynamics. The asymptotic behaviour, which apparently depends on excitation properties involved in physical systems, appears to show the following two distinctive situations: (i) the function $F(t)$ decays to zero as $t \to \infty$ whether slowly or fast; (ii) it does not decay to zero but approaches nonzero (a finite value). Symbolically, (i) and (ii) imply $\lim_{t\to\infty} F(t) \equiv F(t = \infty) = 0$ and $F(t = \infty) \neq 0$, respectively. The spectral distribution of the function contains a delta function singularity at the origin, $\delta(\omega)$, because of $F(t = \infty) \neq 0$ for (ii), while it does not for (i).

The time evolution between (i) and (ii) is essentially different. The presence of the singularity $\delta(\omega)$ (localized excitation) gives rise to a drastic change in the kinetic properties. To be specific, let us consider for example the time evolution of a wavepacket moving in a large system. Then the propagation can be characterized by the following dynamical quantities: the probability of finding a particle at time t, the inverse variance of the wavepacket, etc. The probability, for example, tells us that if there is a localized state induced in a system due to

scatterers (e.g. impurities), then a quantum particle's motion belonging to the localized state will be limited to some finite region so that the probability of finding this particle does not vanish, giving a nonzero chance to be found for $t \to \infty$. However, if a quantum particle propagates on a perfect lattice in which only extended states are present, it simply delocalizes throughout the whole lattice, resulting in zero chance. In general, these quantities mentioned above are expected to decay like a power-law form $t^{-\alpha}$ for a sufficiently long-time limit. Then the propagation exhibits delocalization if $\alpha > 0$ (i.e. $F(t = \infty) = 0$) and localization if $\alpha = 0$ (i.e. $F(t = \infty) \neq 0$) [1].

Suppose, as another example under consideration, that a many-particle system is properly perturbed, where $F(t)$ is a correlation function of a dynamical variable, e.g. a tagged particle position. Then a plausible interpretation in the situation (ii) is that although time evolves the correlation function does not decay any further but remains at a nonvanishing value beyond a certain time window, which reflects a sort of feedback process: an amount of the perturbation energy delivered to the system is returned or remains so that we cannot remove the energy permanently from the tagged particle, resulting in the nondecay of the correlation function.

Perhaps on analysis of a variety of dynamical phenomena a transition between the above two situations is likely to occur. In this context, it may be interesting and important to examine the underlying asymptotic behaviour of the dynamical quantity on a theoretical basis.

Our fundamental concern in this paper is as follows. If $F(t)$ undergoes a transition between the two situations, then how does its structure change between the short-time region and the long-time one, and is there a certain condition on $F(t)$ that governs the transition? Furthermore, how can one discriminate whether $F(t = \infty) = 0$ or $\neq 0$? This discrimination is, however, usually very difficult without knowledge of $F(t)$ for a sufficiently long-time regime. Moreover, for many-particle or complex systems, evaluating $F(t)$ up to such a regime may not be feasible due to real computational constraints. Therefore, it may be necessary to pursue the idea that $F(t = \infty)$ can be extracted or predicted from finite time (i.e. $t < \infty$) knowledge of $F(t)$.

The dynamical function $F(t)$ can usually be investigated via a power series or a continued fraction (CF) representation [2–5]. The power series expansion analysis shows a difficulty which is briefly mentioned in the following section. Hence, we consider the CF representation for our study. The main point considered here is to take coefficients of the CF expansion as basic elements for describing the dynamical function, and to examine the characteristics of the CF coefficients particularly near the transition. The CF coefficients, which are time-independent (i.e. static) quantities, completely determine the underlying dynamical behaviour. This paper is organized as follows. In section 2, we present a way to study the problems posed above, which is based on the CF representation. We show that the presence of the delta function singularity, $\delta(\omega)$, is intimately related to the structure of the CF coefficients and there exists a convergence condition for the structure. Here each pair of even and odd coefficients plays the key role of convergence. This feature allows us to make prediction possible. In section 3, we apply our approach to various physical systems in which the CF coefficients are calculable, to confirm the validity of our idea. Although the physical systems are different the characteristics of the CF coefficients are found to show a similarity. This result is understood by the condition. Finally, concluding remarks are given in section 4.

2. Theoretical approach

To specify the function $F(t)$, we assume that $F(t)$ (appropriately normalized) has a time-reversal invariance with a real even function, $F(t) = F^*(-t)$, * denoting complex conjugate,

and its short-time expansion exists such that $F(t) = \sum_{k=0}^{\infty}(-1)^k c_k t^{2k}/(2k)!$ with the coefficients (moments) $\{c_k\} \geqslant 0$ where $c_0 = 1$, $F(t = 0) = 1$.

The question here is that if the moments c_k are given up to some order of k, is it then possible to predict $F(t = \infty)$. Analysis of the moments is difficult because c_k become very large as the order k increases and also it is hard to find a connection between $t < \infty$ and $t = \infty$ regimes. Instead, we analyse the function via a continued fraction (CF) representation. If $F(t)$ is Laplace transformed, $\tilde{F}(z) = \int_0^{\infty} \mathrm{e}^{-zt} F(t)\,\mathrm{d}t$, then this Laplace-transformed function may be expanded as a CF form [2, 3]

$$\tilde{F}(z) = \cfrac{1}{z + \cfrac{d_1}{z + \cfrac{d_2}{z + \cfrac{d_3}{z + \cdots}}}} \tag{1}$$

with the CF coefficients $\{d_k\} \geqslant 0$. Here $\{d_k\}$ are functions of $\{c_k\}$. They are connected as follows: $c_1 = d_1, c_2 = d_1 d_{12}, c_3 = d_1\big(d_{12}^2 + d_2 d_3\big), c_4 = d_1\big[d_{12}^3 + d_2 d_3 (d_{12} + d_{1234})\big]$, etc. where the notation $d_{12\cdots l}$ denoting $d_1 + d_2 + \cdots + d_l$ was used. Therefore, if the moments $\{c_k\}$ are given, the CF coefficients $\{d_k\}$ are calculable. The converse is also true, namely that the $\{d_k\}$ are also algebraic functions of the $\{c_k\}$. Note that these coefficients are time-independent (i.e. static) real nonnegative values.

Now, by noting $F(t = \infty) = \lim_{t\to\infty} F(t) = \lim_{z\to 0} z\tilde{F}(z)$ and using the CF equation (1), we readily find

$$F(t = \infty) = \frac{1}{1 + \frac{d_1}{d_2} + \frac{d_1}{d_2}\frac{d_3}{d_4} + \frac{d_1}{d_2}\frac{d_3}{d_4}\frac{d_5}{d_6} + \cdots} \equiv \frac{1}{1 + G}. \tag{2}$$

Here $G = \sum_{n=1}^{\infty} g_n$ where $g_1 = \frac{d_1}{d_2}$, $g_2 = g_1\frac{d_3}{d_4}$, $g_3 = g_2\frac{d_5}{d_6}, \ldots$. Then our posed problem is reduced to inquiring whether the series G is convergent or not. That is, $F(t = \infty) \neq 0$ if $G < \infty$ and $= 0$ if $G \to \infty$. Note that the units of g_n, G, and $F(t = \infty)$ are all dimensionless (pure number) because of the presence of the ratio of d_k having the units of (time)$^{-2}$. Thus,

$$0 \leqslant G \leqslant \infty \qquad 0 \leqslant F(t = \infty) \leqslant 1. \tag{3}$$

The case $F(t = \infty) = 1$ (i.e. $G = 0$) occurs only when $d_1 = 0$. In the frequency ω domain a value $F(t = \infty)$ implies a spectral weight at the origin $\omega = 0$. It is obviously nonnegative as shown in (3).

Let us now consider under which condition the series G converges. Due to the d'Alembert criterion [6], the convergence of the series $G = \sum_{n=1}^{\infty} g_n$ depends upon the following ratio:

$$r \equiv \frac{g_n}{g_{n-1}} \tag{4}$$

that is, the series G is convergent if the ratio $r < 1$ and divergent if $r \geqslant 1$ for $n \to \infty$. It is to be noted that $g_n = \prod_{k=1}^{n} \frac{d_{2k-1}}{d_{2k}}$ and $g_n = g_{n-1}\frac{d_{2k-1}}{d_{2k}}$, and thus the ratio g_n/g_{n-1} then becomes $\frac{d_{2k-1}}{d_{2k}}$. Therefore, the convergence test of the ratio g_n/g_{n-1} for $n \to \infty$ is equivalent to that of the ratio $\frac{d_{2k-1}}{d_{2k}}$ for $k \to \infty$. We point out that d_{2k-1} and d_{2k} correspond to the odd and even CF coefficients, respectively. Here, and in what follows, we will refer to (4) as the convergence condition that we have sought. Each pair of the odd and even CF coefficients shown in equation (2) is successively involved in constructing the asymptotic behaviour of a dynamical quantity. By this pairing nature the possible patterns of $\{d_k\}$ that can yield the convergence behaviour are restricted. For example, it is easy to show from the series G in equation (2) and condition (4) that $\{d_k\}$ with the three repeated elements (a, b, c)

(i.e. $\{d_k\} = \{a, b, c, a, b, c, a, b, c, \ldots\}$) cannot generate the corresponding series G being convergent, regardless of the arrangements of (a, b, c) (namely (a, c, b), (b, a, c), etc). This G always diverges.

Finally, our task is simply to calculate d_k (or c_k) up to some order of $n = 2k$ for a given system and then examine the convergence condition (4). However, as is mentioned before, the calculation is practically limited to some finite order (presumably not large k). We introduce a measure called slope, which is useful in predicting the discrimination with the finite order, defined as

$$S_n = \frac{(\log g_1 - \log g_n)}{(\log 1 - \log n)} \tag{5}$$

with $n \geqslant 2$. This slope has the following property. Consider the onset of transition between $F(t = \infty) = 0$ and $\neq 0$. Then the difference between the slopes S_n with $r \geqslant 1$ and S'_n with $r < 1$, $|S_n - S'_n| \geqslant \epsilon > 0$, may grow as n is increased because of condition (4). Consequently their separation at the transition point is expected to take place. We will illustrate that in the next section. The above-introduced measure is not a unique way to determine the transition but it turns out to be a useful tool at least in our analysis. This usefulness is based on the even and odd features involved in the CF coefficients. In fact, one can see that if some $\{d_k\}$ with the even and odd pattern d_k are chosen, a separation in the slope S_n becomes evident.

To test our approach, we apply it to various physical systems where d_k (and hence c_k) are calculable. These are (A) harmonic oscillators, (B) the Mott–Hubbard transition of the Hubbard model, (C) one-dimensional (1D) spin XY model and (D) quantum propagation of an electron in 1D and 3D tight-binding lattice systems with an impurity and in its 1D system under the action of a dc electric field (Stark ladder). For simplicity, the corresponding F and G will be denoted as F_A, G_A, F_B, etc, and $\{d_k\}$ will be expressed in dimensionless units hereafter.

3. Applications

For (A), the dynamics of a classical coupled harmonic oscillator on a Bethe lattice was studied in [7], where the Hamiltonian is given by $H = (1/2m_0)\sum_i p_i^2 + (k_0/2)\sum_{\langle i,j\rangle}(q_i - q_j)^2$ with the particle mass m_0 and the coupling constant k_0. Here $\langle i, j\rangle$ stands for the nearest neighbour interaction characterized by the coordination number l ($l \geqslant 2$, the case $l = 2$ corresponding to a linear chain lattice), and p_i and q_i represent the particle momentum and coordinate, respectively. Exact solutions for both a velocity autocorrelation function (say, $a(t) = (p_i(t), p_i(0))/(p_i(0), p_i(0))$ with $p_i(0) = p_i(t = 0)$, being the tagged ith particle momentum at initial time $t = 0$) and a memory function (say, $m(t)$) using a CF formalism are shown in [7]. These two functions are connected via the generalized Langevin equation [4] as follow: $\mathrm{d}a(t)/\mathrm{d}t + \int_0^t d_1 m(t - s)a(s)\,\mathrm{d}s = 0$. Its Laplace transformation gives $\tilde{a}(z) = 1/(z + d_1\tilde{m}(z)) \equiv \frac{1}{z+}\frac{d_1}{z+}\frac{d_2}{z+}\cdots$, a CF form, where $\tilde{a}(z)$ and $\tilde{m}(z)$ are the Laplace transformed functions of $a(t)$ and $m(t)$, respectively. Therefore, the velocity autocorrelation function (vaf) is characterized by $\{d_k\}$ with $k \geqslant 1$ and the memory function (mf) by $\{d_k\}$ with $k \geqslant 2$. It has been shown that the CF coefficients with the units of k_0/m_0 for $\tilde{a}(z)$ are given by

$$\{d_k\} = \{l, 1, l - 1, 1, l - 1, 1, l - 1, \ldots\}. \tag{6}$$

Let us examine the series G_A. For the vaf case, we find from the CF pattern $\{d_k\}$ (6) that $\frac{d_1}{d_2} = l$ and $\frac{d_{2k-1}}{d_{2k}} = l - 1$ for $k \geqslant 2$. Hence the ratio r is greater than and equal to 1 (i.e., $r \geqslant 1$) for all k because of $l \geqslant 2$. It follows from condition (4) that the series G_A is divergent and thus $F_A(t = \infty) = 0$. Consequently the vafs of the Bethe lattice ($l > 2$) and

the linear chain ($l = 2$) decay to zero, which is confirmed by the exact results (power-law decays $\sim t^{-3/2}$ and $\sim t^{-1/2} \to 0$ as $t \to \infty$, respectively). The perturbed energy imparted to the particle momentum disperses throughout the lattice system and none of the energy comes back or remains so that the correlation functions die out with time.

For the mf case, we find that $\frac{d_{2k-1}}{d_{2k}} = 1/(l-1)$ for all k. The ratio in (4) then becomes $r = 1$ when $l = 2$ and $r < 1$ when $l > 2$. It follows from condition (4) that G_A is divergent for $l = 2$ but convergent for $l > 2$. This convergent case yields a nonvanishing value, $G_A = \sum_{n=1}^{\infty} g_n = \frac{1/(l-1)}{1-1/(l-1)} = 1/(l-2)$. From equation (2) we get $F_A(t = \infty) = 0$ for $l = 2$ and

$$F_A(t = \infty) = \frac{1}{1 + G_A} = \frac{(l-2)}{(l-1)} \neq 0 \tag{7}$$

for $l > 2$. Note that $F_A(t = \infty) < 1$. Consequently, the mf for the linear chain case with $l = 2$ decays to zero while for the Bethe lattice case with $l > 2$ it does not decay to zero but approaches the limiting value (7), which is exactly the same result as obtained in [7]. Note that we simply recovered all the $t = \infty$ limit results without performing the nontrivial inverse Laplace transform, i.e. $F_A(t) = (1/2\pi\mathrm{i}) \int_c \mathrm{e}^{zt} \tilde{F}_A(z)\,\mathrm{d}z$ where $\tilde{F}_A(z)$ implies $\tilde{a}(z)$ or $\tilde{m}(z)$. In the context of the generalized Langevin equation the memory function incorporates all the internal fluctuating processes after the initial perturbation. In the Bethe lattice with $l \geqslant 3$, the fact that there exists no well defined wave vector gives rise to a long-lived fluctuating mode localized at zero frequency in the memory function, which is responsible for the nonvanishing memory, whereas in the linear monatomic chain ($l = 2$) the processes in motion are regular and thus no such localized mode is present. Consequently, they keep losing memory as time progresses, eventually yielding the decay of the memory function to zero.

Let us now look at some numeric values of the slope S_n (equation (5)) for the mf case with $l = 2$ and 3, for instance. Then we see that $S_{n \geqslant 2} =, 0, 0, 0, \ldots$ (constant zero slope) for $l = 2$ and $-1, -1.26, -1.5, -1.72, \ldots$ (increasing negative slope) for $l = 3$, indicating that the separation between the two slopes is persistently getting larger as n increases. Thus this indication tells us that the transition takes place between $l = 2$ and $l \geqslant 3$.

For (B), the Hubbard model the Hamiltonian is given by $H = -\sum_{\langle ij \rangle \sigma} t c_{i\sigma}^{\dagger} c_{j\sigma} + (U/2) \sum_{i\sigma} n_{i\sigma} n_{i,-\sigma}$, where $\langle ij \rangle$ means nearest neighbour sites and $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) is the fermion creation (annihilation) operator with spin σ at site i [8, 9]. In [8], the one-particle Green function given by $F_B(t) \equiv (c_{i\sigma}^{\dagger}(t), c_{i\sigma}(0))/(c_{i\sigma}^{\dagger}(0), c_{i\sigma}(0))$ with $c(0) = c(t = 0)$ on an infinite dimensional Bethe lattice was calculated in the paramagnetic ground state. Its Laplace–Fourier transform called density of states (DOS), $\tilde{F}_B(z)$ with $z = \mathrm{i}\omega + \epsilon$, at the chemical potential $\mu = U/2$ was shown to be written as a CF form, and its CF coefficients were found to be given by

$$\{d_k\} = \{\delta_1, \delta_2, a, b, a, b, a, b, \ldots\} \tag{8}$$

where $\delta_1 = a + \frac{1}{2}b$, $\delta_2 = \left(ab + \frac{1}{4}b^2\right)/\delta_1$, and $a = \frac{1}{4}U^2$ and $b = 2lt^2$, l being a coordination number. We note that this alternating pattern $\{d_k\}$ resembles that of case (A). Let us investigate the series G_B for the DOS. We find from (8) that $\frac{d_1}{d_2} = \frac{\delta_1}{\delta_2}$ and $\frac{d_{2k-1}}{d_{2k}} = a/b$ for $k \geqslant 2$. Then the ratio in (4) becomes $r \geqslant 1$ if $a/b \geqslant 1$ and $r < 1$ if $a/b < 1$. Thus the series G_B is divergent if $a/b \geqslant 1$ and convergent if $a/b < 1$. Its converging value is easily calculated as follows: $G_B = \sum_{n=1}^{\infty} g_n = (\delta_1/\delta_2)\left(1 + \sum_{n=2}^{\infty} (a/b)^{n-1}\right) = (\delta_1/\delta_2)b/(b-a)$. As a result, from equation (2) we obtain that $F_B(t = \infty) = 0$ for $a \geqslant b$ and

$$F_B(t = \infty) = \frac{1}{1 + G_B} = \frac{(b-a)/b}{\delta_1/\delta_2 + (b-a)/b} \neq 0 \tag{9}$$

for $a < b$. Note $F_B(t = \infty) < 1$.

This value (9) is exactly equal to a weight of peak at zero frequency regarded as a measure of quasiparticle mass renormalization obtained in [8] (see equation (30) therein). This peak is due to the Coulomb interaction in the Hubbard Hamiltonian where a particle with different spin state is only allowed to sit on a site. The Mott–Hubbard transition occurs at a critical value U_c (i.e. at $a = b$).

To look at some numeric values of the slope S_n here, consider the cases with $a/b = 1.2$, $a/b = 1$ and $a/b = 1/1.2$. Assuming $\delta_1/\delta_2 = a/b$, we find that $S_{n\geqslant 2} = \{0.26, 0.33, 0.39, 0.45, \ldots,\}$, $\{0, 0, 0, \ldots,\}$ and $\{-0.26, -0.33, -0.39, -0.45, \ldots\}$, respectively, exhibiting that the slopes split at $a = b$ and their splitting becomes wider persistently. This separation indicates that the transition occurs at $a = b$.

For (C), the one-dimensional nearest neighbour coupled spin-$\frac{1}{2}XY$ model Hamiltonian is given by $H = 2\sum_i J\left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y\right)$, where S_i^α with $\alpha = x, y$ are the spin operators at site i. In [10], a spin relaxation function for the XY model given by $F_C(t) \equiv \left(S_i^\alpha(t), S_i^\alpha(0)\right)\big/\left(S_i^\alpha(0), S_i^\alpha(0)\right)$ was calculated via a CF representation, and its CF coefficients were found to be given by

$$\{d_k\} = \{1, 2, 3, 4, 5, \ldots, k, \ldots\} \tag{10}$$

where $d_k = k\delta$ with $\delta = 2J^2$. In this case, we find that $\frac{d_{2k-1}}{d_{2k}} \to 1$ as $k \to \infty$, yielding the ratio $r \to 1$. Thus G_C diverges and $F_C(t = \infty) = 0$. We can also see this divergence in another way: since $G_C = \frac{1}{2} + \frac{1\cdot 3}{2\cdot 4} + \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6} + \cdots$ can be realized by a binomial $(1-x)^{-1/2} = 1 + \frac{1}{2}x + \frac{1\cdot 3}{2\cdot 4}x^2 + \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}x^3 + \cdots$ [6], it follows that $G_C = \lim_{x\to 1}((1-x)^{-1/2} - 1) \to \infty$. The relaxation function thus decays to zero, which is confirmed by the exact result (Gaussian decay $\sim e^{-J^2t^2} \to 0$ as $t \to \infty$). Excitation of a tagged spin regularly transfers throughout the entire neighbouring spins, resulting in no excitation energy to return or stay and thus no $\delta(\omega)$ singularity in the spin relaxation function.

We see that the slope $S_{n\geqslant 2} = -0.415, -0.427, -435, -0.440, -0.444, -0.447, \ldots$. The slope variation becomes very small, approaching a limiting value quickly. This behaviour indicates the divergence of G_C.

For (D), we consider the motion of an electron propagating through a lattice system in the presence of an impurity and/or a dc field. The considered Hamiltonian is given by the tight-binding form

$$H = \sum_i \epsilon_i |i\rangle\langle i| + V\sum_{\langle ij\rangle} |i\rangle\langle j| + eEa\sum_i i|i\rangle\langle i| \tag{11}$$

where $|i\rangle$ denotes the Wannier state of the electron on site i, $\langle ij\rangle$ nearest neighbour interaction, V the hopping energy between i and j, ϵ_i the on-site energy at i, e the charge, E the dc electric field, and a the lattice constant. We assume that one impurity is at site $i = 0$ with the energy ϵ_0 in an otherwise perfect lattice (i.e. $\epsilon_i = \epsilon_0\delta_{0i}$) and an electronic wavepacket initially located at a site i starts to propagate through the lattice. The time evolution is governed by the time-dependent Schrödinger equation $i\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$, where $|\psi(t)\rangle$ is the wavefunction at time t and $\hbar = 1$. The dynamical quantity we want to study here is the following probability (observable): if the wavepacket given above is at the site $i = 0$ at time $t = 0$, what is the probability of finding it at the same site after an infinitely long time $t \to \infty$ has gone? By measuring this probability (which may be said to be the return probability [1]) one can see the effect on the propagation of the wavepacket caused by impurities or electric field. If a lattice is perfect, a particle can evolve to infinity. It is delocalized throughout the lattice. This probability then becomes zero for $t \to \infty$. If, however, the initial site belongs to a localized state due to the impurity or the field, the propagation is confined to a finite region.

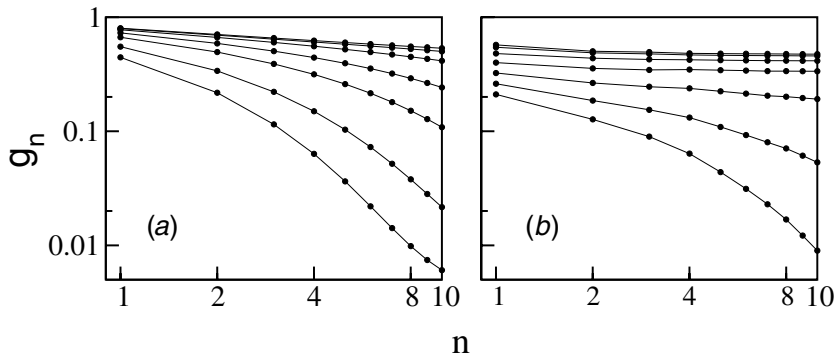

Figure 1. Log–log plot of the g_n versus n for various values of the impurity strength $\overline{\epsilon}$ (from the top to the bottom lines). (*a*) $\overline{\epsilon} = 0.0, 0.2, 0.4, 0.7, 1.0, 1.5, 2.0$ for the 1D system. (*b*) $\overline{\epsilon} = 0.0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0$ for the 3D system.

This probability then becomes nonzero for $t \to \infty$. This probability at arbitrary time t may be written as

$$F_D(t) = |\langle 0|\psi(t)\rangle|^2 \tag{12}$$

where $|0\rangle$ is the initial state of electron on the site $i = 0$ at time $t = 0$. Hence our task here is to see whether $F_D(t = \infty) = 0$ or $\neq 0$.

First, we consider the impurity problem above for the 1D linear chain lattice as well as the 3D simple cubic lattice when the dc electric field is absent, i.e. $E = 0$. We find that the expressions of d_k for $F_D(t)$, equation (12), which is a function of ϵ_0/V, become quite complicated as the order of k increases. We cannot deduce its general pattern as in the cases (A)–(C). Therefore by using a computer we have numerically computed d_k for different values of ϵ_0/V up to $k = 20$ (i.e. ten g_n).

To see the overall behaviour of G_D we draw a log–log plot of the g_n versus n. For the 1D system the results are shown in figure 1(*a*). One can see that each line depends on the impurity strength defined by $\bar{\epsilon} = \epsilon_0/V$. Near $\bar{\epsilon} = 0$ the lines are seen to be rather straight. As $\bar{\epsilon}$ increases they bend down persistently and rapidly. This indicates that they separate from the line for $\bar{\epsilon} = 0$. For the 3D system the results are shown in figure 1(*b*) where we note that even though $\bar{\epsilon}$ increases the lines do not tend to bend down before they exceed a certain $\bar{\epsilon}$. To look at this feature with a finer scale we calculate the slope S_n defined by equation (5). The results are presented in table 1. We find that, as in the cases (A) and (B), they separate at a critical value $\bar{\epsilon}_c$: the slopes decrease (which means they are going towards positive slopes) if $\bar{\epsilon} \leqslant \bar{\epsilon}_c$ while they increase (going more towards negative slopes) if $\bar{\epsilon} > \bar{\epsilon}_c$. Near $\bar{\epsilon}_c$ the slope variations are relatively small but rather fluctuating in the 3D case. We estimate $\bar{\epsilon}_c = 0.1$ (see table 1 and compare between $\bar{\epsilon} = 0.1$ and 0.2) for the 1D case and $\bar{\epsilon}_c = 4.0$ (compare $\bar{\epsilon} = 4.0$ and 4.1) for the 3D case. The transition appears to take place at the critical value $\bar{\epsilon}_c$.

The numerical results of the d_k for the 1D and the 3D systems are depicted in figures 2 and 3, respectively. We observe that the CF coefficients show each pairing of the odd and even d_k illuminating condition (4): for $\bar{\epsilon} \leqslant \bar{\epsilon}_c$ the ratio r approaches 1 rather quickly while for $\bar{\epsilon} > \bar{\epsilon}_c$ r does not become 1, i.e. $r < 1$, as the order k is increased. Let us compare the present case with the previous ones (A) and (B) near the transition. We then find that the characteristics of their CF coefficients are similar, exhibiting an alternating pairing feature. This might be termed 'dynamical similarity' in the sense that the dynamical quantities, even

Table 1. The slope S_n shown for different impurity strength $\bar{\epsilon}$ in the 1D system (the upper section) and the 3D system (the lower section).

S_n(1D)	$\bar{\epsilon}=0$	$\bar{\epsilon}=0.1$	$\bar{\epsilon}=0.2$	$\bar{\epsilon}=0.3$	$\bar{\epsilon}=0.4$	$\bar{\epsilon}=0.5$	$\bar{\epsilon}=0.7$	$\bar{\epsilon}=1.0$	$\bar{\epsilon}=1.5$	$\bar{\epsilon}=2.0$
S_2	−0.180 10	−0.182 73	−0.190 63	−0.203 74	−0.221 99	−0.245 26	−0.306 27	−0.430 63	−0.705 66	−1.029 70
S_3	−0.180 77	−0.183 96	−0.193 52	−0.209 43	−0.231 63	−0.260 06	−0.334 99	−0.488 96	−0.830 84	−1.231 13
S_4	−0.180 24	−0.183 91	−0.194 92	−0.213 28	−0.238 99	−0.272 00	−0.359 43	−0.539 98	−0.940 45	−1.404 51
S_5	−0.179 41	−0.183 51	−0.195 84	−0.216 44	−0.245 36	−0.282 61	−0.381 64	−0.586 74	−1.040 04	−1.554 47
S_6	−0.178 52	−0.183 02	−0.196 58	−0.219 27	−0.251 21	−0.292 45	−0.402 43	−0.630 64	−1.131 42	−1.677 90
S_7	−0.177 65	−0.182 53	−0.197 24	−0.221 91	−0.256 73	−0.301 77	−0.422 21	−0.672 46	−1.214 38	−1.771 13
S_8	−0.176 82	−0.182 06	−0.197 87	−0.224 44	−0.262 01	−0.310 72	−0.441 25	−0.712 60	−1.288 29	−1.832 05
S_9	−0.176 04	−0.181 63	−0.198 49	−0.226 89	−0.267 12	−0.319 38	−0.459 72	−0.751 21	−1.352 59	−1.861 47
S_{10}	−0.175 31	−0.181 23	−0.199 11	−0.229 28	−0.272 10	−0.327 81	−0.477 73	−0.788 30	−1.406 77	−1.865 12
S_n(3D)	$\bar{\epsilon}=0$	$\bar{\epsilon}=3.0$	$\bar{\epsilon}=3.5$	$\bar{\epsilon}=3.8$	$\bar{\epsilon}=4.0$	$\bar{\epsilon}=4.1$	$\bar{\epsilon}=4.3$	$\bar{\epsilon}=4.5$	$\bar{\epsilon}=5.0$	$\bar{\epsilon}=6.0$
S_2	−0.183 88	−0.168 75	−0.219 06	−0.259 89	−0.291 18	−0.307 96	−0.343 64	−0.381 95	−0.487 42	−0.726 92
S_3	−0.132 54	−0.133 81	−0.179 67	−0.228 40	−0.253 17	−0.271 22	−0.310 53	−0.353 92	−0.478 28	−0.775 75
S_4	−0.122 36	−0.101 82	−0.144 82	−0.187 69	−0.223 97	−0.244 44	−0.289 96	−0.341 34	−0.492 58	−0.862 84
S_5	−0.108 68	−0.095 09	−0.141 36	−0.188 92	−0.229 85	−0.253 15	−0.305 36	−0.364 79	−0.541 35	−0.973 99
S_6	−0.100 52	−0.090 41	−0.138 07	−0.188 46	−0.232 57	−0.257 90	−0.315 13	−0.380 87	−0.577 94	−1.063 21
S_7	−0.093 18	−0.088 31	−0.137 37	−0.189 69	−0.235 93	−0.262 67	−0.323 48	−0.393 92	−0.607 45	−1.113 92
S_8	−0.088 45	−0.083 24	−0.130 75	−0.182 96	−0.230 17	−0.257 83	−0.321 61	−0.396 60	−0.628 23	−1.214 27
S_9	−0.084 52	−0.079 38	−0.126 57	−0.180 11	−0.229 50	−0.258 77	−0.326 88	−0.407 79	−0.660 03	−1.297 08
S_{10}	−0.081 09	−0.076 32	−0.123 23	−0.177 86	−0.229 13	−0.259 80	−0.331 78	−0.417 98	−0.688 64	−1.369 59

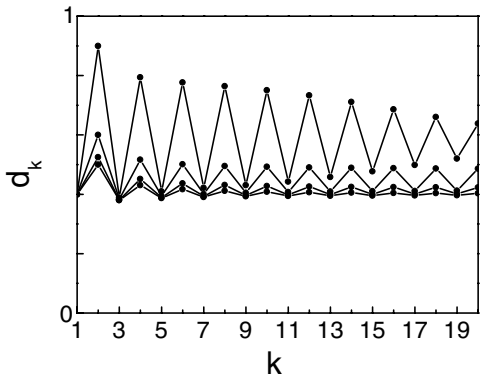

Figure 2. Trends of CF coefficients d_k in arbitrary units versus k for the 1D system are shown for different values of $\overline{\epsilon} = 0.0, 0.5, 1.0, 2.0$ (from the bottom to the top lines). The alternating trend of each pair of the odd and even d_k becomes more pronounced as $\overline{\epsilon}$ is increased. The case with $\overline{\epsilon} = 0.0$ (the bottom one) shows that the alternating trend dies out quickly as k is increased, yielding the ratio $r \to 1$.

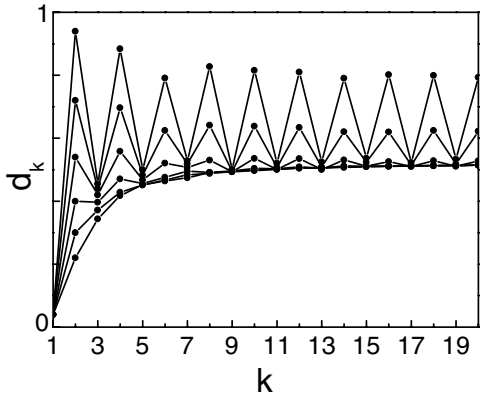

Figure 3. Trends of CF coefficients d_k in arbitrary units versus k for the 3D system are shown for different values of $\overline{\epsilon} = 0.0, 2.0, 3.0, 4.0, 5.0, 6.0$ (from the bottom to the top lines). The alternating trend of each pair of the odd and even d_k begins to show up around $\overline{\epsilon} = 4.0$, and becomes more pronounced for $\overline{\epsilon} > 4.0$. For the cases with $\overline{\epsilon} \leqslant 4.0$ such a trend is hardly seen and the ratio r approaches 1 rapidly as k is increased.

though their physical systems are different, are described by asympotically similar trends of d_k in the long-time limit.

Based on the above results, we can arrive at the conclusion that G_D converges (i.e. $F_D(t = \infty) \neq 0$) for $\bar{\epsilon} > \bar{\epsilon}_c$ and diverges (i.e. $F_D(t = \infty) = 0$) for $\bar{\epsilon} \leqslant \bar{\epsilon}_c$. Hence a localized state due to the impurity exists if $\bar{\epsilon} > \bar{\epsilon}_c$ while no localized state is present if $\bar{\epsilon} \leqslant \bar{\epsilon}_c$. It turns out that our localization problem is equivalent to the problem of finding a bound state induced by an impurity which was studied by Koster and Slater [11, 12]. They used a Green function method to find the corresponding critical values. These are zero for the 1D system and $2/0.4990$ ($\simeq 4.008$) for the 3D system. Our results ($\bar{\epsilon}_c = 0.1$ and 4.0) are in good agreement with their results.

Next, we consider the same problem as above but in the 1D system without the impurity when the dc field $E \neq 0$. The results for a log–log plot of the g_n versus n are shown in

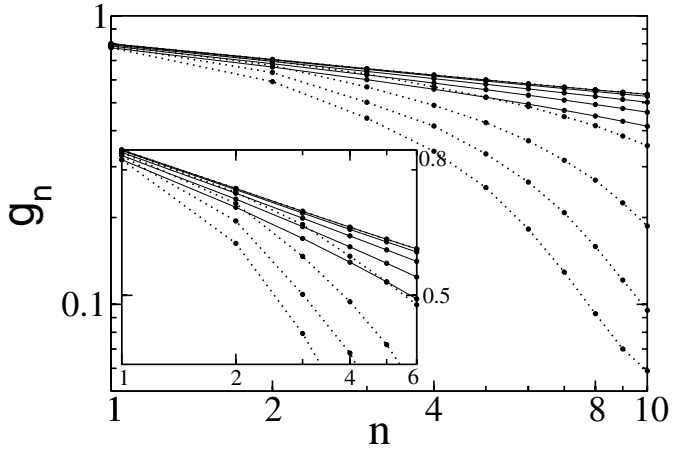

Figure 4. Log–log plot of the g_n versus n for different values of $\overline{E}(\bar{\epsilon}) = 0.0, 0.1, 0.2, 0.3, 0.4$ (from the top to the bottom lines). The dotted lines are for $\overline{E}$ and the solid lines for $\bar{\epsilon}$ in the 1D case. The inset shows magnification near g_n for smaller n.

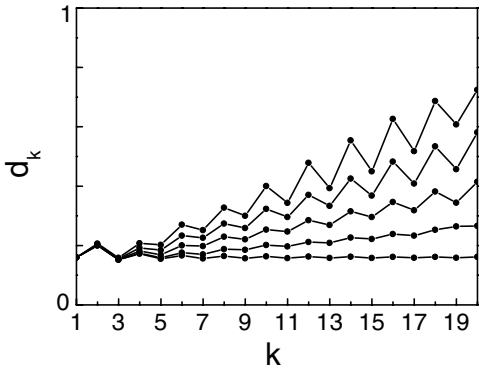

Figure 5. Trends of CF coefficients d_k in arbitrary units versus k for the 1D system with electric field $E \neq 0$ are shown for different values of $\overline{E} = 0.0, 0.1, 0.2, 0.3, 0.4$ (from the bottom to the top lines). The alternating trend of each pair of the odd and even d_k is manifest as the order k as well as $\overline{E}$ are increased.

figure 4 where the field strength is defined by $\bar{E} = eEa/V$. It is well known that the field gives rise to Bloch oscillations and the corresponding critical field strength $\bar{E}_c = 0$ [13, 14]. We observe that the separations (the bending-down of the lines) take place for even smaller $\bar{E}$ compared to the corresponding $\bar{\epsilon}$ for the 1D impurity case. We have examined the slope given by equation (5) to estimate $\bar{E}_c = 0.01$. It is even closer to zero than the impurity's $\bar{\epsilon}_c = 0.1$. In figure 5 the numerical results of d_k are displayed. Here the same pairing features as shown in the preceding cases are observed and reflect condition (4). The d_k in this case are, however, growing with the increasing order of k, which contributes to the rapid convergence of G_D. This implies that the field more strongly induces localized states in the system than the impurity. We have also studied the case where both the field and impurity are present (i.e. $E \neq 0$ and $\epsilon_0 \neq 0$). In this case we find that the additional impurity leads to a more rapid separation for a given $\bar{E}$, indicating that a more pronounced localization occurs in the system [15].

Finally, let us see what happens if the impurity strength $\bar{\epsilon}$ or the field strength $\bar{E}$ is strong. G_D then converges so quickly that the first few g_n become effectively dominant (see g_n for large $\bar{\epsilon}$ and $\bar{E}$ in figures 1 and 4). Thus $G_D < 1$ and from equation (2) $F_D(t = \infty) \simeq 1 - G_D$. In the extreme limit $\bar{\epsilon}$ ($\bar{E}$)$\rightarrow \infty$, then $G_D \ll 1$ and the probability $F_D(t = \infty) \rightarrow 1$. This implies that the electron remains around the starting site, i.e. it gets no chance to propagate to the neighbouring sites. An analogy is the case when it is trapped in a potential well.

4. Concluding remarks

In this paper we have presented a theoretical approach to study the asymptotic long-time ($t \rightarrow \infty$) behaviour of a dynamical quantity $F(t)$. We have found that first, the two asymptotic limits of $F(t = \infty) = 0$ and $\neq 0$ are directly related to the structure of the CF coefficients that is characterized by an odd and even pairing feature, and secondly, the transition between the two limits is determined by the convergence condition of this structure. In addition, this fact allows us to predict its critical point effectively by introducing the slope S_n as an indicator of its separation. The pairing nature following the convergence condition (4) underlies the dynamical similarity.

The important point is that this similarity appears if there are constraints in the systems by which excitation transfers are influenced, although their detailed properties are different. As illustrated in section 3, the constraints turn out to be the lattice structure, interaction, perturbations like impurity and electric field, etc. This suggests that the similarity might not rely on the specific details of systems as far as the asymptotic limits characterized by the CF coefficients are concerned, and also it would be typical in a sort of feedback mechanism. We are planning to present more reports on such a universal feature. We point out that since our theory itself (more specifically the convergence condition itself) is model-independent it can be applied to arbitrary dynamical quantities with a time-reversal invariance. The present study might provide useful information or a basis to explore and understand the transition problems which will appear in general systems.

Acknowledgment

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