Anderson localized state as a predissipative state: Irreversible emission of thermalized quanta from a dynamically delocalized state

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(Received 25 June 2001; revised manuscript received 15 November 2001; published 2 April 2002)

It was shown that localization in one-dimensional disordered (quantum) electronic system is destroyed against coherent harmonic perturbations and the delocalized electron exhibits an unlimited diffusive motion [Yamada and Ikeda, Phys. Rev. E 59, 5214 (1999)]. The appearance of diffusion implies that the system has potential for irreversibility and dissipation. In the present paper, we investigate dissipative property of the dynamically delocalized state, and we show that an irreversible quasistationary energy flow indeed appears in the form of a “heat” flow when we couple the system with another dynamical degree of freedom. In the concrete we numerically investigate dissipative properties of a one-dimensional tight-binding electronic system perturbed by time-dependent harmonic forces, by coupling it with a quantum harmonic oscillator or a quantum anharmonic oscillator. It is demonstrated that if the on-site potential is spatially irregular an irreversible energy transfer from the scattered electron to the test oscillator occurs. Moreover, the test oscillator promptly approaches a thermalized state characterized by a well-defined time-dependent temperature. On the contrary, such a relaxation process cannot be observed at all for periodic potential systems. Our system is one of the minimal quantum systems in which a distinct nonequilibrium statistical behavior is self-induced.

DOI: 10.1103/PhysRevE.65.046211 PACS number(s): 05.45.—a, 72.15.Rn, 71.55.Jv, 71.23.—k

I. INTRODUCTION

Localization problem has attracted much interest for many years [1,2]. Scaling theory of localization suggests that the dimension of disordered systems is directly related to the nature of localization [3]. In two-dimensional disordered system (2DDS) the localization length is much enhanced in comparison with the one-dimensional disordered system (1DDS), but the localization is not still destroyed. In three-dimensional disordered systems (3DDS) there exists the mobility edge in the energy domain above which the localized state is spatially extended. From quantum dynamical and statistical points of view, the state that appears after the destruction of the localized state, which may be called the delocalized state to distinguish from coherently extended state such as the Bloch state, seems to support a complex motion. In other words, the delocalized system, whose eigenbases are almost delocalized, seems to provide with one of the simplest examples of quantum deterministic systems that allow complex stochastic behaviors [4], but its quantum dynamical and quantum statistical properties have not been so extensively investigated. The reason will be that, unlike the localized state to which the renormalization-group-type technique is applicable, it is essentially difficult to devise any theoretical ideas to clarify the delocalized state. Further, the 3DDS that exhibits a typical delocalization do not allow precise numerical studies if the system size is taken large enough to investigate the fully extended states.

If we can design some more simple and numerically accessible systems that exhibit localization and delocalization behaviors, the study of delocalization behavior will be much more advanced. One class of such examples are the one-dimensional incommensurate potential systems that have been studied extensively by a number of authors [5–7].

Another class of systems may be introduced by shifting our viewpoint: the spatial dimension of the disordered systems is nothing more than the number of degrees of freedom, which implies that we may construct a class of systems exhibiting localization and delocalization behaviors by adding new dynamical degrees of freedom instead of increasing the spatial dimension [8–11]. Based upon such an idea, we introduced the 1DDS that is perturbed by the time-dependent harmonic force containing several number of frequency components [11–14]. In our model the number of colors, i.e., the number of different frequencies, can be interpreted as the number of additional degrees of freedom, because the system can be mathematically transformed into the 1DDS coupled with the quantum linear oscillators oscillating at the same set of frequencies [11,13]. We succeeded in demonstrating that transition between localized state and the delocalized state really occurs by changing the number of frequency components and/or the perturbation strength [14]. A great advantage of our system is that it is essentially a one-dimensional quantum system that allows a very long time scale numerical computations with an extreme numerical accuracy, and is very convenient for the quantum statistical and dynamical studies for delocalized state [15].

The time-dependent perturbation itself provides a realistic physical mechanism that much influences the localization properties. Thouless first supposed that the dynamical pertur-
bations by phonons break the localization and brings about diffusion even in strongly localized systems such as 1DDS [16]. An electron, which has a well-defined momentum in the initial stage, loses its memory on the momentum and finally moves like a Brownian particle. However, it has not been very clear what kind of dynamical perturbation destroys the localization mechanism and results in a stationary diffusion in the disordered systems.

If we suppose that the perturbation is due to the phonons composed of infinitely large number of modes, the perturbation must be an incoherent stochastic force with a finite correlation time. It seems quite natural that the incoherent force destroys the quantum coherence that is necessary for the emergence of localization effect. Indeed some authors proposed analytically soluble stochastic models of 1DDS, but the realized diffusion is controlled only by the nature of the stochastic perturbation and is not significantly influenced by the nature of localization [17,18].

In the previous paper [14], we demonstrated that the incoherent perturbation is not necessary for the localization effect to be destroyed: a coherent harmonic perturbation that contains more than one frequency components, i.e., more than one phonon modes, is sufficient for the destruction of the localization. Under such a simple dynamical perturbation, the electron exhibits an unlimited diffusive motion, and the diffusion constant is related to the localization length as was predicted by Thouless provided that the perturbation strength is weak enough. This fact implies that Anderson delocalization mechanism is converted into a diffusion mechanism with the help of only a small number of dynamical degrees of freedom. Our system is a deterministic quantum system with a few degrees of freedom that is isolated from the external world. Appearance of diffusion in our system implies that the dynamically perturbed electron of 1DDS “spontaneously” acquires irreversible dynamical properties without introducing any dynamical randomness from the external world.

Similar phenomena are known also in classically chaotic quantum dynamical systems that exhibit chaotic diffusion in the classical limit. In the quantum systems, the classical chaotic diffusion is suppressed by the localization mechanism, but the diffusion is restored by coupling these systems with each other at a classically negligible very weak coupling strength [19,20].

Appearance of diffusion in 1DDS means that if the electron initially has a definite momentum it can lose the momentum through the interaction with the dynamically perturbed irregular scatterers. However, it is not sufficient for the stationary conduction of electron to be realized. The kinetic energy initially possessed by the electron should also be dissipated as heat. Just this energy dissipation problem is the subject of the present paper.

In the traditional theory of transport phenomena, it is implicitly and/or explicitly supposed that the electronic system is coupled with a heat reservoir [21–26]. The electron loses the momentum that it gained through the acceleration process, by the impurity scattering, and in the next step the excess energy is absorbed by the heat reservoir. In the first step of the impurity scattering the electron loses the phase memory, and the energy relaxation to the reservoir takes place in the second step. Under such a situation, the absolutely continuous spectrum of the infinite number of degrees of freedom composing the heat reservoir plays an essential role in the occurrence of irreversible energy transfer from the electron to the reservoir [27]. In other words, the irreversibility is caused by the loss of dynamical memory due to the absolutely continuous spectrum of the reservoir [28]. In this situation the quality of the energy emitted to wards the reservoir is not considered. The excess energy is surely absorbed by the reservoir, but we cannot have any information to answer the question: does the energy flow in the form of heat or in some other form of energy such as radiation that is convertible to work?

The aim of the present paper is to demonstrate that only a small number of degrees of freedom is sufficient for the occurrence of diffusion (the first step) and energy relaxation (the second step) in 1DDS. We couple the delocalized 1DDS perturbed by a harmonic perturbation with a simple test quantum system that is prepared in its ground state, and show that the delocalization of the electron results in an irreversible quasistationary energy transfer from the electron to the test system. Onset of similar irreversible energy transfer in systems with a few degrees of freedom was studied in detail by one of the present authors for a class of classically chaotic quantum systems [29], and it was shown that under appropriate conditions quantum map systems can absorb energy stationarily without any quantum recurrence. An important result in the present paper is that, in addition to the emergence of irreversible energy transfer, we obtain a strong evidence that the energy transfer occurs in the form of a heat flow. In short, the delocalized electron dissipates the excess energy in the form of heat; delocalization, dissipation, and heat being the three keywords of the present paper. Therefore, the 1DDS coupled with a small number of degrees of freedom provides a minimal deterministic quantum dynamical system that models the whole process of nonequilibrium energy transport in electronic systems.

The outline of the present paper is as follows. In Sec. II model systems investigated in the present paper are introduced. The model we treat here is a one-dimensional tightly binding electron system on irregular or regular on-site energies. In the former case the system is 1DDS that exhibits Anderson localization, whereas the latter case models the Bloch electron. The system is further coupled with harmonic perturbation containing a few frequency components. Such a system is equivalent to an autonomous (i.e., time-independent) quantum system in which the harmonic perturbations are transformed into linear quantum oscillators with the same set of frequencies. Furthermore, we briefly review the phenomenon called the dynamical delocalization, which was observed numerically in the above-mentioned harmonically perturbed 1DDS and was extensively studied in our previous paper.

In Sec. III, we propose the simple test that we call dissipation test to investigate dissipative property of any quantum system, which is done by coupling the quantum system to be tested with a simple test system such as a harmonic oscillator.
that is prepared in a ground state. Further in Sec. III, we examine the dissipation test for the 1DDS driven by polychromatic harmonic perturbations. It is shown that under this condition the system is delocalized if the excess energy initially stored in the electronic system is transported irreversibly to the test system in the form of a quasistationary one-way flow.

In Sec. IV, results of the dissipation test for periodic potential system are given and compared with the result of 1DDS. The energy flow exhibits a recurrent behavior and no one-way flow of energy can be observed in the periodic system.

In Sec. V, we focus our attention to the quantum statistics of the test system, and it is demonstrated that the statistical distribution of test system very promptly approaches Boltzmann-type distribution characterized by a well-defined on-site energy of electron at the site number of harmonic oscillators, and the third one is the 1DDS perturbed by harmonic perturbation and coupled with quantum harmonic oscillators.

A. Nonautonomous model

We consider a tightly binding Hamiltonian $H_j(t)$ for the 1DDS perturbed by classical driving forces oscillating at the mutually incommensurate frequencies $\{\Omega_j\}$.

$$H_j(t) = H_{el} + H_{osc,t}(\{\Omega_j\}),$$  \hspace{1cm} (1)

$$H_{el} = \sum_{n=1}^{N} |n\rangle V(n) \langle n| + \sum_{n}^{N} (|n\rangle \langle n+1| + |n+1\rangle \langle n|),$$ \hspace{1cm} (2)

$$H_{osc,t}(\{\Omega_j\}) = \sum_{n=1}^{N} \sum_{j=1}^{L} \epsilon_j \cos(\Omega_j t) V(n) |n\rangle \langle n|. \hspace{1cm} (3)$$

The basis set $\{|n\rangle\}$ is an orthonormalized one and $V(n)$ is the on-site energy of electron at the site $n$, which varies at random in the range $[-W,W]$ from site to site and the transfer energy vanishes unless the sites are adjacent.

The time-dependent nonautonomous system can be transformed into a time-independent autonomous system. As the autonomous counterpart of the model (1), we consider the autonomous Hamiltonian

$$H_j^{aut} = H_{el} + \sum_{j=1}^{L} \Omega_j J_j + H_{osc,t}(\{\phi_j\}), \hspace{1cm} (4)$$

where the source of the external harmonic perturbation in the model (1) is taken into account by the linear oscillators described by the angle variable operators $\phi_j$ and their conjugate action variable operators

$$J_j = -i\hbar \frac{\partial}{\partial \phi_j}. \hspace{1cm} (5)$$

Then it follows that the time-evolution unitary operator of the autonomous system is related to the unitary time-evolution operator of the autonomous system

$$\exp\left\{-iH_j^{aut}t/\hbar\right\} = \exp\left\{-i \sum_{j=1}^{L} \Omega_j J_j t/\hbar\right\} \times \hat{T} \exp\left\{-i \int_{0}^{t} ds H_j(\Omega_j s + \phi_j)/\hbar\right\}, \hspace{1cm} (6)$$

where $\hat{T}$ means time-ordering operator. If we take the eigenstate of the angle operators with the eigenvalue $\phi_{j0}$ as the initial state of the linear oscillator, then the action of the evolution operator of the autonomous model is equivalent to that of the original nonautonomous model perturbed with the harmonic force with the initial phases $\phi_{j0}$.

It is well-known that almost all the eigenstates are exponentially localized in 1DDS without the perturbation (i.e., $\epsilon_j = 0$) [1]. The finite localization length means that if the initial wave packet is spatially localized, the wave packet does not spread over the space, and the memory on the initial wave packet do not disappear. In other words, there are no stochasticization process that result in any statistical behavior, and the 1DDS is not ergodic and, of course, does exhibit no mixing property, i.e., no decay of correlation. Such features may be, however, drastically changed if the localized system is perturbed by the harmonic forces $\{\cos(\Omega_j t)\}$ [12–14]. We will give a brief summary of the nonautonomous system in Sec. II B, which describes the key features to understand the motivation of the present paper.

For the sake of simplicity, $\epsilon_j$ common values are taken for the perturbation parameters, such that

$$\epsilon_j = \frac{\epsilon}{\sqrt{L}}, \hspace{1cm} (7)$$

in the present paper, and the parameter $\epsilon$ characterizes the perturbation strength.

B. Dynamical delocalization in nonautonomous system

In our previous paper [14] we showed that the 1DDS exhibits a remarkable delocalization behavior when it is perturbed by classical oscillating forces with several frequency components. Since such a delocalization phenomenon is a
key to understand the occurrence of irreversibility and dissipation that are the main subjects of the present paper, we review it rather in detail.

When oscillatory harmonic perturbations are applied to 1DDS, an initially localized wave packet of electron \( |\Psi(t = 0) = \delta_{t,0} \rangle \) spreads unlimitedly, and we called such a quantum state dynamically delocalized state. It is very interesting that such a nonlocalized state can be easily realized only by applying a weak coherent perturbation. The delocalization property can be quantitatively characterized by the mean square displacement (MSD) of the wave packet: \( m_2(t) = \langle \Psi(t) | r^2 | \Psi(t) \rangle \), where \( \hat{r} = \sum_{n=1}^{\infty} n|n\rangle \langle n| \) is the position operator and \( \Psi(t) \) is the time-dependent wave packet.

It is found that the wave packet, which is localized without the interaction with the oscillatory perturbation, spreads beyond the original localization length as time elapses. The diffusive behavior is observed within the time scale accessible by numerical computations, and the diffusion process is not in general the normal diffusion but a subdiffusion, which is characterized by a power law increase,

\[
m_2(t) \sim t^\alpha \quad (0 < \alpha \leq 1).
\] (8)

The subdiffusive behavior approach the normal diffusion \( (\alpha = 1) \) promptly as the number \( L \) of the frequency and/or the perturbation strength \( \epsilon \) increase. However, we note that in the monochromatic case \( (L = 1) \) the diffusive behavior is suppressed at a certain level that is much longer than the original localization length. We investigate the property of the delocalized states in the following sections.

C. Autonomous model

Let us consider the model of the 1DDS coupled with finite number of harmonic oscillator modes with incommensurate frequencies \( \{ \omega_j \} \),

\[
H_{\text{II}} = H_{\text{el}} + H_{\text{ph,M}} + H_{\text{int,M}},
\] (9)

where \( H_{\text{ph,M}} \) represents the harmonic oscillator Hamiltonians

\[
H_{\text{ph,M}} = \sum_{j=1}^{M} \left( \frac{\hat{p}_j^2}{2} + \omega_j^2 \hat{q}_j^2 \right),
\] (10)

and the interaction Hamiltonian with coupling strength \( \{ b_j \} \) is given by

\[
H_{\text{int,M}} = \sum_{n=1}^{N} \sum_{j=1}^{M} |n\rangle V(n) \langle n| b_j \hat{q}_j.
\] (11)

Physically such additional harmonic oscillators can be looked upon as the phonon modes that perturb the electronic system, and so we often call them "phonon modes." By using the creation and annihilation operator of Fock states of the harmonic oscillators, the interaction Hamiltonian is rewritten as

\[
H_{\text{int,M}} = \sum_{n=1}^{N} \sum_{j=1}^{M} |n\rangle V(n) \langle n| \beta_j (a_j^\dagger + a_j) \sqrt{\frac{\hbar \omega_j}{2}},
\] (12)

where \( \beta_j = b_j / \omega_j \).

Now we make clear the relation between the two models \( H_{\text{II}}(t) \) and \( H_{\text{II}} \). To this end, we consider the extreme case in which all the phonon modes are excited around the Fock states with large quantum numbers, \( N_j^\pm (j = 1, 2, \ldots M) \). Then only the Fock states close to such states are relevant for the interaction process, and the matrix elements of the interaction Hamiltonian can be looked upon as a constant because

\[
\langle N_j^+ + n_1, \ldots, N_j^+ + n_m | H_{\text{int,M}} | N_j^+ + n'_1, \ldots, N_j^+ + n'_M \rangle
\]

\[
\approx \sum_{n=1}^{N} \sum_{j=1}^{M} |n\rangle V(n) \langle n| b_j \sqrt{\frac{\hbar \omega_j}{2}} \delta_{n,n'^j} \delta_{n,n'^j 1},
\] (13)

for \( n_j, n'_j << N_j^+ \). Under the approximation, the autonomous system \( H_{\text{II}} \) becomes equivalent to the autonomous counterpart \( H_{\text{II}}^{\text{aut}} \) of the nonautonomous model \( H_{\text{II}}(t) \). Indeed, if we use the action eigenstates of the action operators such that \( J_j|m_j\rangle = m_j \hbar |m_j\rangle \) \( (m_j : \text{integers}) \) as the basis for the model \( H_{\text{II}}^{\text{aut}} \), the phase variable representation of the action eigenstates is given by \( \langle \{ \phi_j \}| m_j \rangle = \Pi_j M_j e^{im_j \phi_j / \sqrt{2 \pi}}, \) and the matrix elements of the interaction Hamiltonian \( H_{\text{osc,L}} \) with respect to the action eigenstate \( \Pi_j M_j |m_j\rangle \), which is given by

\[
\langle \{ m_j \}| H_{\text{osc,L}}(\{ \phi_j \}) | \{ m_j' \} \rangle = \sum_{n=1}^{N} \sum_{j=1}^{L} |n\rangle V(n) \langle n|
\]

\[
\times \epsilon_j \delta_{m_j, m_j' z = 1/2},
\] (14)

is equivalent to \( H_{\text{int,M}} \) under the following identifications:

\[
\{ \langle \{ N_j^+ + n_j \} \} \leftrightarrow \{ m_j \},
\] (15)

\[
\epsilon_j \rightarrow \sqrt{2 b^j N_j^+ \hbar / \omega_j}.
\] (16)

Thus the harmonically perturbed nonautonomous system is equivalent to the autonomous system coupled with harmonic oscillators when all the harmonic oscillators are excited to large-quantum-number states.

If the number of phonon modes goes to infinity with an absolutely continuous spectrum as \( \omega_l \approx \omega_i \), then the phonon system becomes a boson heat bath that has been used as the model of heat reservoir [27], but the number of phonon modes is kept finite throughout our treatment.

D. Mixed model

If some of the harmonic oscillators are highly excited, we can replace them by the time-dependent harmonic perturbation. In this paper we mainly treat with a conventional model in which most of the harmonic oscillators (the number is \( L \)) are replaced by time-dependent harmonic perturbations with the same frequency, but a very few number of oscillators (the number is \( M \)) are in the ground state and so they cannot be
Hamiltonians

We solve the Schro"dinger equation for the three sorts of numerically.

discussed in detail in Sec. III. The model Hamiltonian is thus replaced by the time-dependent harmonic perturbation. The ANDERSON LOCALIZED STATE AS A . . . PHYSICAL REVIEW E

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generic nature of the Anderson localized states. In the sense, we can attribute the essential origin of the dissipation to the Anderson-localized state very weakly, becomes dissipative, oscillatory perturbations, is

is a single electron system coupled with a small number of delocalized systems discussed in the previous section, which

exceptional examples in classically chaotic quantum systems [29].

What we wish to show in this section is whether or not the delocalized systems discussed in the previous section, which is a single electron system coupled with a small number of oscillatory perturbations, is dissipative in the above sense. If the localized state, which is realized by perturbing the Anderson-localized state very weakly, becomes dissipative, we can attribute the essential origin of the dissipation to the generic nature of the Anderson localized states. In the sense, the Anderson-localized state is a predissipative state as is

used in the title of the present paper.

A. Technical remarks

In the present case the quantum system S consists of an electron and oscillatory perturbation, which is represented by the Hamiltonian H (t). In order to investigate whether the system is dissipative or not, we set the test mode at the ground state and couple it with S. Since we use a harmonic oscillator as the test mode, the whole system relevant for the dissipation test is equivalent to the mixed model H III of L \geq 2 and M = 1 introduced in Sec.II D.

First we examine the dissipation test with the Anderson-localized 1DDS without any oscillatory perturbation (L = 0-system). Second, we try the dissipation tests for dynamically delocalized states that are observed in L \geq 2-systems.

The key parameters controlling the dissipation test are the frequency \omega (= \omega) and the coupling strength, b (= b). In our simulation the parameter \hbar \omega is chosen as 0.1, and Planck constant is fixed. The periodic boundary condition is imposed on both electron and the test phonon mode in order to apply the fast Fourier transformation, where the site number of electron and the number of meshes of the test mode are taken typically N = 128 and N ph = 64, respectively. We did not take the ensemble average over different configurations of the disordered system because of the limitation of our computer power. We mainly used 60 000 step, i.e., the total time T = 1500.

We prepare the electron initially in a highly excited state, and compute the time-dependent electronic energy E_{el}(t) = \langle \Psi(t)|H_{el}|\Psi(t)\rangle, MSD and the energy stored in the test mode, i.e., E_{ph}(t) = \langle \Psi(t)|H_{ph,M}|\Psi(t)\rangle, by the time-dependent wave packet \Psi(t). We number the localized eigenstates of the isolated 1DDS from the top of the energy levels and denote the number by n_j. We mainly use the third eigenstate (n_j = 3) as the initial state of the electron system.

B. Unperturbed case (M = 1, L = 0)

In this section, we examine the dissipation test for isolated 1DDS by coupling it with a harmonic oscillator, which is taken as T. Since the system S is Anderson localized in the present case, we may expect that there is no dissipation when S is coupled with T. However, an interesting problem in the present case is whether the back action from the excited T itself works for the localized electron like an oscillatory perturbation and may significantly change the localization properties.

The time dependence of electronic energy and phononic energy of the test mode together with MSD of electron are respectively displayed in Figs. 1(a,b,c) for several values of b and the fixed value \omega = 0.8. In this case the energy of the total system is conserved and the decrease in the electronic energy transfers to the increase of the phononic energy. At a very weak coupling strength (b = 0.2), there is no significant transfer of energy from the electron to the phonon. But as the coupling strength exceeds a critical level (b \sim 0.5), the transferred energy to the phonon suddenly increases, and at relatively strong coupling strengths (b \sim 0.9 and 1.1) the energy of electron decreases monotonically, and so the energy emitted to the phonon mode T does not return to the electron system. The energy transferred from the excited electron is almost stored in the phonon mode (see Fig. 2). Correspondingly, the wave packet also spreads suddenly from the original Anderson-localization length to the level comparable to the system size. We can interpret that such a type of transition is due to the self-induction of the oscillatory perturbation by T. In this sense it seems that the system S attains a dissipative property above the threshold, but the decrease in the electronic energy is not complete and does not reach the zero level. This fact implies that the achieved dissipation is not still complete. Correspondingly, the growth of MSD de-
Picted in Fig. 1 terminates at the level smaller than the system size, and so the localization length is drastically enhanced but the localization is not still destroyed. As a result, we can conclude that the electron energy irreversibly flows to the phonon mode if the coupling strength exceeds a critical value, but the flow of the energy saturates before the system reaches a fully relaxed state.

C. Polychromatically perturbed case \((M=1, L>2)\)

In this section we examine dissipation test for the polychromatically perturbed 1DDS. When the number of the frequency components of the perturbation is larger than or equal to 2 \((L\geq2)\), the 1DDS exhibits typical sign of dynamical delocalization. Note that monochromatically perturbed 1DDS cannot show the delocalized behavior although the localization length is enhanced [14]. The dissipation test for the monochromatically perturbed 1DDS is given in Appendix A.

Typical examples of time-dependent energy transfer between a polychromatically perturbed system \((L=5)\) and the test mode are depicted in Figs. 3 and 4. Figure 3 shows the time-dependent features observed at various values of perturbation \(\epsilon\) with the fixed coupling strength \(b=0.4\), whereas Fig. 4 shows the results at various values of \(b\) with the fixed perturbation strength \(\epsilon=0.4\).

In all cases the MSD grows up to the maximum scale and so a complete delocalization is achieved, and the electronic energy shows a very nice relaxation behavior. In the early stage of time evolution, the electron loses its energy linearly in time, which is observed as the linear increase of the phononic energy. In such a quasistationary regime the emission rate of energy per unit time can be well defined. Monotonic increase of phonon energy continues until the wave packet spreads over the system size and the electronic energy approaches zero level, which indicate a complete delocalization.

It seems that the dissipative nature is not lost even at very small \(\epsilon\), but the energy transfer rate depends linearly on \(\epsilon\) if \(\epsilon\) is small enough. It is also proportional to the coupling constant \(b\).

In conclusion, all the above features indicate that a complete dissipation is realized in case of \(L>2\).

Finally, we overview the \(L\) dependence of the time-dependent behavior in Fig. 5. It is evident that as the number \(L\) of the frequency components increases, the localization is destroyed and simultaneously a nice one-way transfer of energy from the electron to the phonon appears. In the limit of \(L\to\infty\) the “oscillatory” perturbation becomes a random force, and it seems to be no wonder that such a stochastic
perturbation destroys the localization phenomenon that is just a manifestation of quantum coherence. Indeed, we show in Appendix B 1 that very similar results are obtained in the dissipation test of stochastically perturbed 1DDS. However, we have to emphasize that only a small number of different frequencies is sufficient for the system to exhibit complete delocalization and complete dissipation.

FIG. 3. Time dependence of (a) an electronic energy, (b) a phononic energy, and (c) MSD of electron in polychromatically perturbed cases ($L=5$), where $W=0.9$, $h=1/8$, $b=0.4$, $\omega=0.8$, and various perturbation strengths $\varepsilon=0.1, 0.2$, and 0.4. The frequency components of the perturbation $\{\Omega_i\}$ are chosen within a range $[0.5, 1.5]$ randomly.

FIG. 4. Time dependence of (a) an electronic energy, (b) a phononic energy, and (c) MSD of electron in polychromatically perturbed cases ($L=5$), where $W=0.9$, $h=1/8$, $\varepsilon=0.4$, $\omega=0.8$, and various coupling strength $b=0.2, 0.4, 0.8, 1.1$. The frequency components of the perturbation $\{\Omega_i\}$ are chosen within a range $[0.5, 1.5]$ randomly.

IV. DISSIPATION TEST CASE OF BLOCH STATES

If the on-site energy of electronic system varies periodically, the electron is in Bloch states that are fully extended over all the sites on the one-dimensional lattice. We may expect quite different dissipation property for such periodic systems. In this section we examine the dissipation test to Bloch electron in periodic systems and compare the results with those of the delocalized system investigated in the previous sections.

First we consider the simplest periodic case in which all the on-site energies $V_n$ are the same. Then the total system, consisting of the electronic part and the test harmonic oscillator, becomes separable, thus the test system $T$ does not couple with the electron system. We, therefore, consider a binary periodic system, in which the on-site energy varies periodically as $V_n=W$, $V_{n+1}=-W$, $V_{n+2}=W$, $V_{n+3}=-W \ldots$ from site to site.

A. Monochromatically perturbed case ($M=1$, $L=1$)

We perturb the binary periodic 1D electron system with a monochromatic perturbation and regard it as $\mathcal{S}$. It is evident
that such a system is not separable when it is coupled with the \( T \) mode, and energy in general transfers between \( S \) and \( T \).

The time dependence of electronic and phononic energies together with MSD of electron are respectively displayed in Fig. 6. The figure shows the energy recurs between \( S \) and the test mode \( T \), which is initially prepared in the ground state. Furthermore, such properties of the time dependence does not depend on whether the time-dependent oscillatory perturbation \((L = 1)\) exists or not.

**B. Polychromatically perturbed case \((M = 1, L \geq 2)\)**

The essential behavior of the time dependence is almost the same as monochromatically perturbed case except for periodic pattern of the recurrence. The energy oscillates between electron and the test mode, and net energy transfer cannot be observed even in the cases where we use many frequency components (see Fig. 7).

However, if the polychromatic perturbation is replaced by a stochastic perturbation, which corresponds to the limit \( L \to \infty \), the energy transfer from electron to the test mode is observed, and the test system can absorb energy from electronic state, where the absorption rate increases approximately proportional to the perturbation strength. This is a quite natural result that the random force externally introduced destroys the quantum coherence that yields the quantum recurrence. The result is given in Appendix B 2.

As a result we cannot observe any one-way energy transfer between the perturbed spatially periodic system and the test mode: the electron and the \( T \)-phonon mode exchange...
energy quasiperiodically over all the time scale. We may thus conclude that spatial irregularity of the on-site energy is essential for the onset of dissipation.

V. STATISTICAL PROPERTY OF TEST MODE

In the original sense of dissipation, the irreversible transport of energy is not sufficient condition for the onset of dissipation. More precisely, a dissipation process is taking place if the two features are observed: (*1) a one-way flow of energy occurs from $S$ to $T$, and, (*2) the energy is transported in the form of a heat flow. In the present section, we pay attention to quantum state of the harmonic oscillator as other degrees of freedom during the time evolution.

A. Dissipation and Boltzmann-type distribution

In this section we return to the dissipation test for the periodically perturbed 1DDS. The polychromatic perturbation destroys Anderson localization, and a one-way transfer of energy occurs from the delocalized system if the system is coupled with another degree of freedom $T$, which is taken as a harmonic oscillator mode in our simulation. Such a process can be regarded as a spontaneous emission of quanta (phonons) generated by a radiation source composed of the electronic degree of freedom. Roughly speaking, the quasistationariness of the irreversible emission of phonons will be attributed to the decoherence of the radiation source, which is self-generated through the interaction process of the 1DDS with the oscillatory perturbation. It is of great interest to investigate the quantum statistical property of the radiated quanta.

First we show in Fig. 8 the case of a polychromatic perturbation ($L = 5$) that exhibits a typical dynamical delocalization. The semilog plots of probability distribution with respect to the Fock space $P(E_{n_{ph}}) = |\langle n_{ph}|\Psi(t)\rangle|^2$ of the test phonon mode versus the eigenvalue of energy $E_{n_{ph}}$ are depicted at several time steps, where $|n_{ph}\rangle$ is the number state of the phonon mode. A remarkable fact is that the plots all ride on a straight lines very well, and so the distribution in the Fock space is well fitted by the Boltzmann-type distribution characterized by the time-dependent temperature $T(t)$,

$$P(E_{n_{ph}}) \propto \exp\left(-\frac{E_{n_{ph}}}{T(t)}\right).$$

We show in Fig. 9 that the off-diagonal element $P(m_{ph},n_{ph}) = |\langle m_{ph}||\Psi(t)\rangle\langle\Psi(t)||n_{ph}\rangle|^2$ decays quickly in time and finally exhibits a rapidly fluctuating motion around zero, which vanishes if averaged over a longer time scale.

Figure 10 shows the time-dependent temperature evaluated by the data in Fig. 8. The phonon temperature $T(t)$ rises in accordance with the energy of the test phonon mode, and when the phononic energy saturates the temperature also reaches an equilibrium temperature. When the polychromatic perturbation is replaced by a stochastic perturbation, a similar Boltzmann-type distribution can also be observed. The result is given in Appendix B 1. In this way, the polychromatic perturbation composed of only finite number of frequency components gives rise to the same effect as the stochastic perturbation. On the other hand, the Boltzmann-like statistics of the $T$ mode is not observed when the oscillatory perturbation contains less than two frequency components and the
system $S$ does not exhibit a complete delocalization. Figure 11 shows such an example. Indeed, the semilog plot of the distribution function significantly deviates from the straight line of the Boltzmann-type distribution.

We can therefore conclude that the emergence of complete dissipation is obviously correlated with the formation of the Boltzmann-type distribution in the test phonon mode.

**B. Generality of thermalization**

Why the Boltzmann-type distribution emerges when the system is dissipative? We can give a simple phenomenological interpretation. To the end, we derive the Heisenberg equation of motion for the annihilation operator $a(t)$ of the $T$ mode:

$$\frac{da(t)}{dt} = -i\omega a(t) + R(t),$$

where the term $R(t)$, given by

$$R(t) = -ib \sqrt{\frac{\omega}{2\hbar}} \sum_n U(t)|n\rangle \langle n| U^\dagger(t),$$

As is described in Sec. III, the phonon number increases in proportion to $t$ in the initial stationary stage, which can be explained by supposing that the correlation function $\langle R^\dagger(t_2)R(t_1)\rangle = \Phi(t_1, t_2 - t_1)$ depends weakly on $t_1$ and decays very rapidly as time interval $|t_2 - t_1|$ exceeds a short characteristic time $t_c$. Neglecting the weak dependence of the correlation function on $t_1$, the expectation value of $T$ increases in proportion to time,

$$\langle a^\dagger a \rangle = t \int_0^\infty e^{-i\omega s} \Phi(s) ds.$$

Further, from Eq. (20), $a^\dagger$ is an integration over the stochastic source with the very short characteristic time $t_c$. The amplitude $a^\dagger$ is a sum over statistically independent quantities and hence should obey a Gaussian stochastic process [22]. Regarding $a^\dagger$ as a number, the distribution function of $a^\dagger$ should be the Gaussian distribution $P(a, a^\dagger) \propto \exp[-\text{const} \times |a|^2]$, which is equivalent to the Boltzmann-type distribution.

Therefore it seems that the thermalization together with the quasistationary emission of phonons is a manifestation of a rapid destruction of quantum coherence, which is represented by the decay of correlation. If the above interpretation is true, the origin of the Boltzmann distribution is due to the fact that the field amplitude is expressed by an integration over the stochastic source, which happens as a result of the particular choice of the system $T$. Indeed, if we choose an
anharmonic oscillator instead of the harmonic oscillator as the test system, the integral relation (22) do no longer holds correct, and the statistics of \( T \) may significantly deviate from the Boltzmann-type distribution.

To answer the question we examined a simulation in which the harmonic oscillator is replaced by an anharmonic oscillator. We take the quartic oscillator that does not have the harmonic potential components as the test system \( T \):

\[
H_{ph,M=1} = \frac{\hat{p}^2}{2} + \hat{q}^4.
\]

We may expect that the statistics of the quartic oscillator deviates significantly from the Boltzmann-type distribution even though the correlation of the source term decays promptly. We show in Fig. 12 a typical example of the semilog plot of the probability \( P(E_n) = |\langle n_{ph}\psi(t)\rangle|^2 \) for a significant energy range, where \( |n_{ph}\rangle \) and \( E_{n_{ph}} \) are the \( n_{ph} \)th eigenstate and its energy, respectively. Contrary to the first expectation, the plot is again almost on a straight line, which indicate that the distribution of \( T \) obeys the Boltzmann-type distribution even in case of the quartic oscillator. Figure 13 shows the time dependence of the energy stored in the quartic oscillator. It again shows a nice linear growth until the saturation effect due to the finite available energy becomes significant. These facts imply that the thermalization effect cannot be attributed to the combined effect due to the linearity of the test mode \( T \) and the rapid decay of correlation in the radiation source.

We still do not have a definite physical idea to explain such distinct features, but we will argue on a possible underlying mechanism in the following section.

C. Anderson localized state as a pre-dissipative state

In the course of the emission of quanta into the mode \( T \) the energy of \( T \) increases as if the system has a well-defined temperature, and the temperature rises from zero to some finite value \( T(t) \). The only natural way to prepare a simple integrable system \( T \) in a thermalized state is to couple the initial \( T \) at zero temperature virtually with a heat reservoir having the same temperature \( T = T(t) \) and infinitely large heat capacity. If the whole system, i.e., reservoir+\( T \) is ergodic, the quantum statistics of \( T \) should approach the Boltzmann distribution. In the process through which \( T \) approaches an equilibrium state with the heat reservoir, the energy is transported from the reservoir to \( T \) in the form of “heat.” The fact that temperature is well defined for \( T \) means that the transfer of energy from the electron to the mode \( T \) occurs in the form of “heat.” In short we are allowed to interpret that the electronic energy is dissipated as heat.
The autonomous version of the Hamiltonian of the total system $S$ play the role of a "reservoir" for $T$ such that the system $S$ relaxes to the thermalized state. Namely, the system $S$ may form a quantum ergodic system. Then it is quite natural that the system $T$ is described by Boltzmann-type distribution, because $T$ forms a relatively small subsystem of the ergodic system. The essential problem is whether or not the interaction between the electron and the oscillators enables a global connection between the unperturbed quantum states, which will be strongly correlated with the occurrence of delocalization. We note further that $S$ is composed of only a small number of degrees of freedom and do not have infinitely large heat capacity. Further detailed studies along the idea mentioned above will be reported elsewhere $[30]$. Anderson localization is destroyed even by a very weak interaction with a few dynamical degrees of freedom, which is simulated by polychromatic perturbation in the present paper, and it releases the stored energy as "heat." This is the very reason why we termed Anderson-localized state a "pre-dissipative" state in the title of the paper. We emphasize here again that our system is a small deterministic quantum system. The "heat" has been considered as a macroscopic concept connected with the loss of microscopic information to control the associated system. It will be of fundamental interest to investigate how the concept of heat can be extended to microscopic quantum systems. Our system provides with an example to study the fundamental problem.

VI. SUMMARY AND DISCUSSION

Dissipation property of 1DDS perturbed by time-dependent harmonic driving force, which exhibits a remarkable delocalization behavior, is numerically investigated by coupling the system with another simple system prepared in the ground state. We have regarded that the system is dissipative if an irreversible transfer of energy occurs from the electronic system to the test system in the form of a one-way energy flow. It has been demonstrated that the dynamically perturbed 1DDS is dissipative when the electron is completely delocalized, and moreover the quantum statistics of the test system becomes Boltzmann distribution with a well-defined time-dependent temperature. The latter fact allows us to interpret that the energy transferred from the 1DDS is dissipated as heat. The complete dissipation takes place when the number of frequency component is more than one and a complete delocalization occurs in the polychromatically perturbed 1DDS.

Dissipative behavior is not observed at all if the 1DDS is replaced by periodic potential systems that have Bloch eigenstate. The energy transferred to the test system changes quasiperiodically around the zero level, and no net energy is dissipated as heat.
transfer can be observed. The spatial irregularity in the potential plays a critical role in the actualization of dissipation and also delocalization.

The origin of the irreversibility may be attributed to the complexity in the phase relation peculiar to the localized eigenfunction \cite{31,28}. The localization is dynamically destroyed even by weak dynamical perturbations, and the phase complexity manifests itself, resulting in dissipation and delocalization. In this sense the localized state can be regarded as a pre-dissipative state. The potential for mixing and dissipation in localized systems resembles the characteristics of classically chaotic quantum systems \cite{32,29}. Indeed, as discussed in Introduction, a quantum chaos system also exhibits dissipative behavior under a very weak coupling with dynamical perturbations \cite{29}. Chaos provides a promising mechanism that can create sufficient complexities to induce an apparently irreversible behavior in closed quantum systems. As is demonstrated in the present paper, spatial irregularity can also be an origin of quantum irreversibility in systems with a small number of degrees of freedom. In particular, the thermalization effect is a quite new result that has not still been reported in quantum chaos systems. It will be of interest to explore whether similar thermalization do occur also in quantum chaos systems that exhibit dissipative behavior.

We may expect that our idea might be extended to the delocalized state in the 3DDS. In this case, the localized state is already destroyed above mobility edge without the coupling taking place with any other dynamical degrees of freedom. If we prepare the electronic system in an energetically...
excited state and couple it with the test system, then it might be expected that the stored electronic energy is spontaneously and irreversibly converted into heat and flows into the test system. If this is the case, the 3DDS is the minimal deterministic quantum system in which dissipation and thermalization are self-organized. Thus far, the localization/delocalization phenomena have not been explicitly investigated from the viewpoint of dissipation and thermalization. The significance of dissipation and thermalization in small deterministic quantum systems must be investigated more extensively.

It is expected that such kind of studies become important in statistical physics of systems with a few degrees of freedom such as mesoscopic device [33–36], molecular machine systems [37], quantum computer [38] and so on [39–41]. In particular, investigation of the meaning of heat and dissipation in microscopic quantum system will be of fundamental importance when we evaluate the upper bound of efficiency and controllability of microscopic quantum devices.

**ACKNOWLEDGMENT**

The authors express thanks to Dr. Shoji Tsuji for his hospitality in providing a location for our discussions, where important progress in the idea of the present paper was made.

**APPENDIX A: MONOCHROMATICALLY PERTURBED CASES (M=1, L=1)**

In this appendix we observe how the dissipative property of the 1DDS changes by applying a monochromatic oscillatory perturbation to the system. As has been discussed in Sec. II B, the additional monochromatic perturbation enhances the localization length, and therefore we may expect that a more complete dissipation will be observed when the system $T$ is coupled with $S$. We may further expect that the

![FIG. 16. Time dependence of (a) an electronic energy, (b) a phononic energy, and (c) MSD of electron in stochastically perturbed cases, where $W=0.9$, $h=1/8$, $b=0.4$, and the perturbation strength $\epsilon=0.2$, 0.3, 0.4, and 0.6.](image1)

![FIG. 17. (a) Increasing rate $R_{ph}$ of the phononic energy and (b) diffusion rate $D$ of the localized electron estimated by data in Fig. 16, as a function of the perturbation strength.](image2)
test mode $T$ itself plays the role of an additional perturbation, and the total system becomes equivalent to a dichromatically perturbed 1DDS in which an unlimited diffusion takes place [14]. However, if the coupling between $S$ and $T$ is weak enough, the $T$ mode is not well excited, and the self-induced perturbation is not strong enough to destroy the localization completely.

In fact, as shown in Fig. 14, when the coupling strength $b$ is small enough ($b = 0.1$), the growth of MSD does not reach the level of the system size and the localization still remains. The increases in the phonon energy, which are shown in Figs. 14(a,b), also terminate as the electron energy stops to decrease and in turn begin to increases before reaching the zero level. Figure 14 also shows examples of MSD at larger perturbation strength ($\varepsilon = 0.2$ and 0.4). Delocalization and

FIG. 18. Phonon distribution $P(E_{\text{phon}}) = |\langle n_{\text{phon}} | \Psi \rangle|^2$ at several times ($t = 100, 200, 300, 400, 500$) in stochastically perturbed 1DDS. The parameters are $b = 0.4$ and $\varepsilon = 0.4$.

FIG. 19. Time dependence of (a) an electronic energy, (b) a phononic energy in stochastically perturbed binary periodic system, where $W = 0.9, \ h = 1/8, \ b = 0.3, \ \varepsilon = 0.2, 0.3, \text{and} 0.5$.

FIG. 20. Increasing rate $R_{\text{phon}}$ of the phononic energy estimated by data in Fig. 19 as a function of the perturbation strength.

FIG. 21. Phonon distribution $P(E_{\text{phon}}) = |\langle n_{\text{phon}} | \Psi \rangle|^2$ at several times ($t = 100, 200, 300, 400, 500$) in a stochastically perturbed binary periodic system. The parameters are $b = 0.3$ and $\varepsilon = 0.2, 0.3, \text{and} 0.5$. 

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transfer of energy from electron to phonon seem to continue on a longer time scale, and an apparently one-way energy transfer occurs from $S$ to $T$. However, the electron does not emit all the possible energy. In this sense the system becomes partially dissipative but a complete relaxation of energy is not still realized.

On the other hand, as shown in Fig. 15, if the coupling strength is large enough ($b = 1.0$) the diffusion and a one-way energy transfer continues until it reaches a fully relaxed state even at smaller values of perturbation strength. The MSD also approaches the maximum length allowed by the finite system size ($m_s \sim 1400$). The final electronic state with almost zero energy can be regarded as an equilibrium state that contains all the localization bases, whose energies are distributed symmetrically around zero, with even statistical weight. We can judge that the system is delocalized and becomes completely dissipative in such a coupling strength regime. The flowing rate of energy increases in accordance with the increment in the perturbation strength $\epsilon$.

In conclusion, if the coupling strength is small enough, the localization is not still destroyed and the irreversible energy relaxation takes place partially. On the other hand, as the coupling between $S$ and $T$ becomes strong, a complete delocalization and a complete dissipation are both realized.

**APPENDIX B: DISSIPATION TEST FOR STOCHASTICALLY PERTURBED CASES**

In this appendix we summarize results of dissipation test for stochastically perturbed delocalized and Bloch states in disordered and binary periodic systems, respectively.

1. Disordered system

Figure 16 shows time dependence of the energy in the cases of the stochastically perturbed localized state for various perturbation strength. In comparison with the polychromatically perturbed cases with the same perturbation strength $\epsilon = 0.4$ in Fig. 10, we can see that the effect of the polychromatic perturbation ($L \geq 4$) are almost the same as that of the stochastically perturbed one. In the stochastic cases, $E_{ph}$ increases and $E_{el}$ decreases linearly until the states are fully relaxed. Generally, we may say that the quasistationary energy transfer from electron to the test phonon mode occurs in strong connection with the delocalizing behavior.

The increasing rate $R_{ph}$ of the phononic energy of the test mode is shown in Fig. 17(a) as a function of the perturbation strength, and Fig. 17(b) shows the diffusion rate $D$ estimated by the data depicted in Fig. 16(c) for some perturbation strength. With the increase in the perturbation strength, both $R_{ph}$ and $D$ exhibit a clear linear growth.

Figure 18 shows the semilog plots of the probability distribution in the Fock space of the test phonon mode, which is measured at several time steps. Apparently, all the plots ride on straight lines very well. Hence the distribution in the Fock space is also well fitted by the Boltzmann-type distribution.

2. Binary periodic system

Even in cases of Bloch electron a quasistationary one-way energy transfer can be realized by applying stochastic perturbation to the system. Figure 19 shows a result of the energy exchange between the electron and the test mode in cases of the stochastically perturbed Bloch electron. An irreversible energy transfer can be observed: the energy of the phonon mode increases almost linearly. Correspondingly the energy of electron decreases on average, but it is accompanied by a fluctuation around the zero level.

In Fig. 20 we show the increasing rate $R_{ph}$ of the mode energy as a function of the perturbation strength. $R_{ph}$ increases almost linearly in proportion to the perturbation strength.

We recall that in the disordered system the polychromatic perturbation ($L \geq 4$) gives rise to almost the same effect as the stochastic perturbation. On the contrary, in case of the periodic system the polychromatic perturbation brings no irreversible energy transfer, but the stochastic perturbation results in an apparently irreversible behavior although the energy transfer process is accompanied by an enormous fluctuation.

Furthermore, it should be noted that in the case of periodic system the statistical behavior of the phonon mode seems not to be well fitted by the Botzmann-type distribution. Indeed, the distribution fluctuates so violently that the temperature can no longer be well defined (see Fig. 21). It is a remarkable difference from the disordered system.

[4] We use the term “deterministic” system in the sense that the system does not include any time-dependent stochastic perturbation even if it is a disordered system with spatial randomness throughout the present paper. The term “stochastic behavior” is used in the sense that the behavior of time evolution of the state is similar to one in a stochastically perturbed 1DDS.