Energy relaxation dynamics in a quasi-periodic system coupled with a small number of phonon modes

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Abstract

Energy relaxation dynamics in the Harper model coupled with a small number of phonon modes is numerically investigated. In the case of the Harper model irreversible energy transport between the electron and the phonon mode, which have been observed in the case of disordered systems, can be observed independent of the potential strength. In the irreversible energy flow, the role of the localization or randomness can be confirmed in comparison to the results in a periodic or disordered system. The coherent state representation of an autonomous phonon mode during the relaxation of the energy are also shown to confirm the process of phase randomization. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction and model

There have been some attempts at examining quantum dissipation [1]. In the orthodox approaches, stochastization mechanisms are explicitly or implicitly assumed in advance. A more interesting scenario of the electronic stochastization is the possibility that the stochastization mechanism is spontaneously organized in the system without any help from the external stochastic source. Indeed, it has been shown that just few phonon modes are sufficient for an irreversible energy transfer from the scattered electron to an autonomous phonon mode to be induced if the scattering potential is spatially irregular [2,3]. On the other hand, the energy relaxation could not be observed for Bloch electron in a periodic system [4]. We are interested in whether this kind of irreversible phenomena can be observed in the case of the Harper model or not, in which both localized states and extended states can be easily realized by change of the potential strength. In the present paper we investigate the effect of localization and randomness of the electronic system on the energy relaxation by means of the Harper model.

The time-dependent Shrödinger equation that we simulate is

\[
\frac{i\hbar}{\partial t} \Psi(n, \{q_j\}, t) = \Psi(n + 1, \{q_j\}, t) + \Psi(n - 1, \{q_j\}, t)
\]
In Fig. 1 the time dependences of the energy $E_{el}(t)$ and $E_{ph}(t)$ are shown for some cases with a localized initial state ($V_0 > 1$). In the unperturbed case ($\varepsilon = 0$), the energy relaxation occurs, but the flow saturates at a certain level, i.e., it is not a complete relaxation. In the perturbed case ($\varepsilon \neq 0$), the energy relaxation continues until the electrons fully relax at the equilibrium level. The whole structure of the energy transfer in the Harper system is almost similar to that in the disordered system [2,4]. Fig. 2 shows the result in the case of the system with extended states ($V_0 < 1$). It is found that the energy relaxation structure is almost similar to the localized case in Fig. 1, and it is quite different from cases of Bloch states in periodic systems [4].

As a result the time-dependent behavior of $E_{ph}(t)$ and $E_{el}(t)$ do not strongly depend on the property of the eigenstates of the Harper model. Of course, the MSDs are quite different in Figs. 1(c) and 2(c), depending on the potential strength which divides the eigenstates into localized or extended state. It seems that the irreversible energy transfer is brought about only by irregularity of the potential sequences. It is very interesting to note that such a nonequilibrium statistical behavior can be observed in a simple closed quantum system.

The mixing in electronic state reflect on the phononic state. To observe the phase complexity of the autonomous phonon mode, we check the change of coherent state representation during the time evolution. Fig. 3 shows some snapshots of the coherent state ($V_0 > 1$). As we expected by the energy transfer in Fig. 1, the evaluation of phase complexity becomes slow as time elapses in the unperturbed case. On the contrary, it seems that in the perturbed case ($\varepsilon = 0.4$) as $E_{ph}$ increases the phase complexity also increases. The quantitative characterization of the details of the phase complexity is a future problem.

2. **Numerical results**

We initially set the electron in a highly excited state, and the harmonic oscillator in the ground state of the Fock state, and compute the time-dependent autonomous mode energy $E_{ph}(t) = \langle \Psi(t)|H_{ph}|\Psi(t)\rangle$, electronic energy $E_{el}(t) = \langle \Psi(t)|H_{el}|\Psi(t)\rangle$ and its mean square displacement (MSD) by the time-dependent wave packet $\Psi(t)$.

$$
\sum_{j=1}^{M} \left( \frac{p_j^2}{2} + \frac{m_j^2 q_j^2}{2} \right) 
+ \sum_{n=1}^{N} \sum_{j=1}^{M} b_j V(n) q_j + V(n, t) 
\times \Psi(n, \{q_j\}, t) ,
$$

where the $\Psi(n, \{q_j\}, t)$ represent the wave function of the whole system on a site basis. We use the Harper model $V(n) = 2V_0 \cos(2\pi n)$, where $\omega$ is the inverse golden mean ($\omega = (\sqrt{5} - 1)/2$). It is well known that without any interaction with phonon modes ($\varepsilon = 0, b_j = 0$), i.e., the Harper model, all eigenstates are localized when the potential strength $V_0$ is larger than unity and are extended when $V_0$ is smaller than unity [5].

If the number of autonomous phonon modes coupled with electronic system goes to infinity ($M \rightarrow \infty$) with an analytical frequency spectrum such as $\omega_i \propto \Omega$, then the phonon system becomes a heat reservoir implicitly or explicitly supposed in orthodox theories, but in our treatment the number of phonon modes is finite, i.e., typically $M = 1$. It is known that oscillatory external perturbation, i.e., nonautonomous phonon modes, can be mathematically identified with highly excited quantum harmonic oscillator, i.e., autonomous phonon modes [1,2,4]. Accordingly, we can regard the above model as a *closed quantum system* which is consisting of an electronic system and finite number of harmonic oscillators. The degrees of freedom of the total system is $1 + M + L$. In this simulation we set $M = 1$ and $L = 0$ or 1.

3. **Summary and discussion**

We simulated a time-evolution of a pure state consisting of an excited state in the Harper model and a ground state in a harmonic oscillator.
Fig. 1. Time-dependence of (a) a phononic energy $E_{ph}$, (b) an electronic energy $E_{el}$ and (c) MSD of electron, where $h = \frac{1}{k}$, the perturbation strength $\varepsilon = 0.0, 0.2$ and $0.4$ and the frequencies $\omega_1 = 0.8, \Omega_1 = \sqrt{2}$, for the monochromatically perturbed Harper model ($M = 1, L = 1$) with localized state ($V_0 = 1.1$).
Fig. 2. All the parameters and situations are the same as in Fig. 1, except that the Harper model has an extended state ($V_0 = 0.9$).
Irreversible energy flow from electron to the phonon mode could be observed in the quantum system without any stochastization mechanism.

The relaxation of the energy is characterized by decaying of the time correlation function and factorization of the density matrix. The quantum coherence appears in the off-diagonal term of the

Fig. 3. Some snapshots of the coherent states $|\langle X, P | \Psi_0(t) \rangle|$ of autonomous phonon for cases in the Harper model ($V_0 = 1.1$) with (a) $\epsilon = 0$ and (b) $\epsilon = 0.4$. The intervals (2$\pi$) of the $X$ and $P$ are divided into 50 meshes.
density matrix \( \rho(t) = |\Psi(t)\rangle \langle \Psi(t)| \). If a dephasing mechanism which comes from coupling with the other degrees of freedom work well in the electronic system, the off-diagonal terms decay and properties of the quantum state approach that of the classical ensemble as

\[
\text{tr}(\rho(t)X) = \sum_{n,m}^N \langle n|\rho(t)|m\rangle \langle m|X|n\rangle \\
\rightarrow \sum_{n}^N \rho_{nm}(t)X_{nn}.
\] (3)

Thus the off-diagonal matrix element vanishes in the sense that the expectation value of an arbitrary class of operator \( X \) can be well approximated by the diagonal sum only. In this system decay of the velocity–velocity correlation function and the off-diagonal elements of \( \rho(t) \) are the interesting future problems.

References