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Spontaneously induced irreversible energy transport in closed electron–phonon systems

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Abstract

Energy relaxation dynamics associated with the electron scattering process is investigated with a simple fully quantum model of an electron–phonon system. It is numerically demonstrated that contrary to traditional theories infinite numbers of phonon modes are not necessary and just a few phonon modes are sufficient for an irreversible energy transfer from the scattered electron to the phonon modes to be induced if the scattering potential is spatially irregular. Moreover, the phonon mode reaches promptly a thermalized state characterized by a well-defined temperature. The possibility that such a process might be an origin of resistivity in a closed quantum system is discussed.

It is nearly 40 years since the methods for computing electrical resistivity or conductivity have been established as linear response theories [1–3]. In spite of the great success of these theories, the conditions for the occurrence of irreversible energy transfer from electrons to some other degrees of freedom, which is inevitable when an electron accelerated by an applied field is to reach a stationary state, are not fully understood. Conventional theories suppose implicitly or explicitly the presence of a heat reservoir composed of an infinite number of degrees of freedom such as phonon modes. Once we suppose an absolutely continuous spectrum for the heat reservoir, it becomes an energy sink, and the whole system can be regarded as an *open system*. Thus it is not surprising that scattering of electrons naturally yields a one-way energy transfer from the electronic system to the reservoir. It is in such a situation that traditional formulas such as the Kubo formula [1] or the Landauer formula [3]

allow us to compute transport coefficients. Indeed, the validity of the Kubo formula for conductivity has been proved rigorously for a weakly dissipative Lorentz model [4]. A basic question arising here is whether a macroscopic number of degrees of freedom is really necessary for an apparently irreversible energy transfer to be realized in a *closed quantum system*.

The aim of the present paper is to demonstrate that contrary to traditional theories only a small number of phonon modes are sufficient for an irreversible stationary energy transfer from the scattered electron to phonon modes to take place under some appropriate conditions. This fact implies that a stationary one-way transfer of energy can be realized within a closed quantum system with a small number of degrees of freedom isolated from any energy sink or heat reservoir.

There have been some attempts examining the possibility of occurrence of dissipation in closed quantum systems. Most results give negative answers, be-

cause the quantum interference effects in general suppress the appearance of dynamical decoherence [5–8]. However, it has been pointed out that some classically chaotic quantum systems may exhibit effectively irreversible and dissipative behavior [9]. The origin of such an irreversible behavior is attributed to the complexity in the phase structure of chaotic wavefunctions [10].

According to the classical theory of impurity scattering [2], we consider a scattering process by randomly distributed scatterers. The irregularity of the scattering potential tempts the electronic wavefunction to localize, preventing the electronic conduction as a Bloch electron. However, the localized wavefunction has a phase complexity similar to that of a chaotic wavefunction [11]. Therefore, if the localization is destroyed by some mechanism, we can expect that the electronic conduction is recovered and simultaneously the phase complexity still remaining in the localized wavefunction may provide a mechanism leading to a dissipative behavior.

To test the idea we consider a one-dimensional tightly binding electronic system (1-DDS) described by the Hamiltonian

$$H_{el} = \sum_{n=1}^N |n\rangle V(n) \langle n| + \sum_{n \neq m} |n\rangle K(n, m) \langle m|. \quad (1)$$

The basis set $\{|n\rangle\}$ is an orthonormalized one and $V(n)$ is the on-site energy of the 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 n and m are adjacent ($K(n, m) = \delta_{n, m \pm 1}$). The electronic system couples with a small number of phonon modes represented by the harmonic oscillator Hamiltonian with incommensurate frequencies ω_i ,

$$H_{ph} = \sum_{j=1}^M (\frac{1}{2} p_j^2 + \frac{1}{2} \omega_j^2 q_j^2), \quad (2)$$

via the interaction Hamiltonian with coupling strength b_j ,

$$H_{int} = \sum_{n=1}^N \sum_{j=1}^M [|n\rangle V(n) \langle n|] b_j q_j. \quad (3)$$

If the number of phonon mode goes to infinity with an analytical frequency spectrum such as $\omega_i \propto i$, then the

phonon system becomes the heat reservoir implicitly or explicitly supposed in orthodox theories, but in our treatment the number of phonon modes is *finite*, i.e., typically $M = 2$ or $M = 3$. Without the interaction with phonon modes, the electronic wavefunction is Anderson-localized because of the randomness of the on-site potential. However, it may be expected that the coupling with phonons results in a destruction of localization [13].

To gain an insight into the role of phonon modes, we first consider the extreme case in which all the phonon modes are excited around Fock states with a large quantum number, say N_j^* ($j = 1, 2, \dots, M$), then only the Fock states close to $|N_1^*, N_2^*, \dots, N_M^*\rangle = \prod_{j=1}^M |N_j^*\rangle$ are relevant for the interaction process and the matrix element of the interaction Hamiltonian can be considered as a constant,

$$\begin{aligned} &\langle N_1^* + n_1, \dots, N_M^* + n_M | H_{int} | N_1^* + n'_1, \dots, N_M^* + n'_M \rangle \\ &\approx \sum_{n=1}^N \sum_{j=1}^M V(n) b_j \sqrt{\frac{N_j^* \hbar}{2\omega_j}} \delta_{n_j, n'_j \pm 1}, \end{aligned} \quad (4)$$

in the first order approximation ($n_j, n'_j \ll N_j^*$). In this approximation, the original model becomes equivalent to a simple time-dependent Hamiltonian perturbed by a classical driving force oscillating at the frequencies ω_j by using the angle representation of the Fock state [9,14],

$$H_{el}(t) = \sum_{n=1}^N |n\rangle V(n, t) \langle n| + \sum_{n \neq m} |n\rangle K(n, m) \langle m|, \quad (5)$$

$$V(n, t) = V(n) \left(1 + \sum_{j=1}^M \epsilon_j \cos(\omega_j t - \phi_j) \right), \quad (6)$$

where ϕ_j is the angle variable which is taken as a constant and $\epsilon_j = \sqrt{2b_j^2 N_j^* \hbar / \omega_j}$. The phonons perturb the electronic system at multiple frequencies. A remarkable effect of the periodic perturbation is the destruction of localization [16]. This delocalization phenomenon is a key to understanding the occurrence of spontaneous dissipation to be discussed later.

To observe the temporal behavior of the electronic wavefunction in the time-dependent 1-DDS, we monitored the time-dependence of the mean square displacement (MSD) $\langle \Delta n^2 \rangle = \langle \Psi(t) | (\hat{n} - \langle \hat{n} \rangle)^2 | \Psi(t) \rangle$,

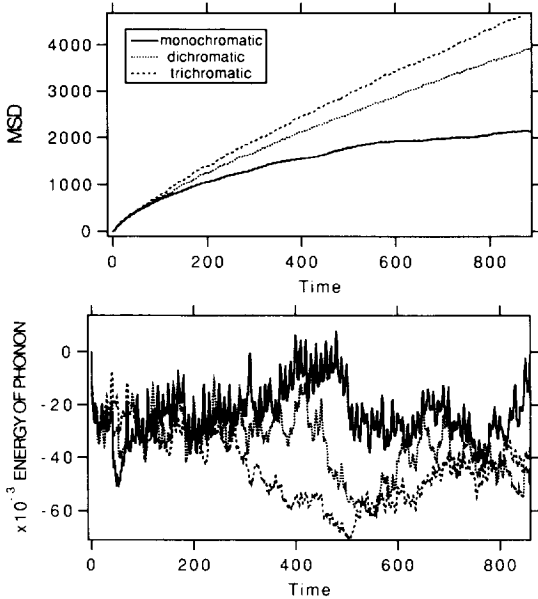


Fig. 1. (a) Time-dependence of mean square displacement of the electron for monochromatic, dichromatic and trichromatic perturbations, where $W = 0.9$ and $\epsilon_j = 0.5$. (b) Time-dependence of phonon energy corresponding to the three cases.

where $\hat{n} \equiv \sum_{n=1}^N n|n\rangle\langle n|$ is the position operator and $\Psi(t)$ is the time-dependent wave packet. The results are shown in Fig. 1a for three types of quasiperiodic perturbation, i.e., monochromatic ($M = 1$), dichromatic ($M = 2$) and trichromatic ($M = 3$). It is found that the wave packet which is localized without the interaction with phonons spreads beyond the localization length as time elapses. The wave packet spreads according to an anomalous diffusion law such that $\langle \Delta n^2 \rangle = Dt^\alpha$ rather than the normal diffusion law, and the exponent α approaches 1 from below as M increases. We call the delocalization phenomenon induced by such a periodic perturbation “dynamical delocalization”.

Fig. 1b shows the energy absorbed by the phonon modes during the time evolution of the packet. It is evident that the absorbed energy fluctuates around the zero level, which strongly indicates that no significant energy transfer occurs between phonons and electron. This is because the phonon diffuses in the ladder of Fock states symmetrically around the initial Fock state with the high quantum number $N_j = N_j^*$. It should be emphasized that the phononic diffusion in the Fock space is a reflection of the electronic diffusion in real

space.

We thus have found that the delocalization of the electronic wavefunction by the periodic modulation of phonon modes surely results in an irreversible diffusion, but there is no energy transfer from the electron. However, if the phonons are initially prepared in their ground states instead of highly excited states, the situation might be drastically changed: suppose that the phonon is set to the ground state of the Fock states, then the diffusion of phonons induced as a back-action of electronic diffusion will occur only in the upper half direction of the Fock space, and the average energy of the phonons should increase, which means that a transfer of energy from electrons to phonons takes place. A problem is that the perturbation to the electron from the phonons in the ground states is only the zero-point vibration due to the quantum fluctuation, accordingly it is questionable whether such a weak and virtual effect can trigger a macroscopic diffusion in both real and Fock spaces.

As the approximation used in deriving the model (5) is no longer applicable when we examine the situation mentioned above, we return to the original model (1) and first examine the monochromatic case ($M = 1$), preparing the phonon in the ground state. To achieve a reliable numerical accuracy, the 6th order symplectic integrator method (typical time step 0.025) was used for the numerical integration of the Schrödinger equation [15]. The periodic boundary condition is imposed on both electron and phonons in order to apply the fast Fourier transformation, where the site number of electrons and the number of the mesh of the phonon system are taken typically $N = 128$ and $N_p = 64$, respectively.

We prepare the electron initially in a sufficiently high excited state, and compute the time-dependent electronic energy $E_{el}(t) = \langle \Phi(t) | H_{el} | \Phi(t) \rangle$ and the phononic energy $E_{ph}(t) = \langle \Phi(t) | H_{ph} | \Phi(t) \rangle$ by the time-dependent wave packet $\Phi(t)$. Before showing numerical results, we briefly comment on the parameters characterizing the electron-phonon interactions. The interaction Hamiltonian (3) can be represented by using creation and annihilation operators of the Fock state, i.e., $H_{int} = \sum_{n=1}^N \sum_{i=1}^M [|n\rangle V(n) \langle n|] \beta_i (a_i^\dagger + a_i) \sqrt{\frac{1}{2} \hbar \omega_i}$, where $\beta_i = b_i / \omega_i$. Thus the interaction strength is characterized by two kinds of parameters, β_i and $\hbar \omega_i$. The

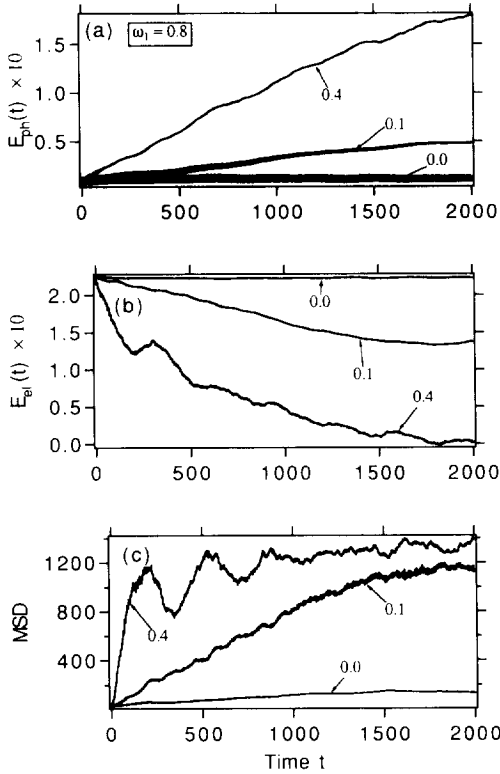


Fig. 2. Time-dependence of (a) electronic energy, (b) a phononic energy and (c) mean square displacement of the electron, where $W = 0.9$, $\hbar = \frac{1}{8}$, the perturbation strength $\epsilon_2 = 0.0, 0.1, 0.4$ and the frequency $\omega_2 = 2\sqrt{2}$. The energy axes are scaled by $\hbar\omega_1 = 0.1$.

latter parameter $\hbar\omega_1$ is chosen to be 0.1 from the observation that the electronic diffusion of the model (5) becomes maximal at this value [16].

The time dependence of electronic and phononic energies together with the MSD of the electron are respectively displayed in Figs. 2a, 2b and 2c as the case of $\epsilon_2 = 0.0$. We can see that the electron and phonon do not exhibit any significant exchange of energy between them. Moreover, Fig. 2c tells us that the diffusion of the initially localized wave packet of the electron is very weak. The above facts manifest that the zero-point fluctuation of a phonon in the ground state is not strong enough for a significant mixing to occur in the electronic system.

We may expect that the electronic mixing is much enhanced by adding another phonon mode to the system ($M = 2$). To achieve an efficient mixing, the second phonon mode should be fully excited. Under

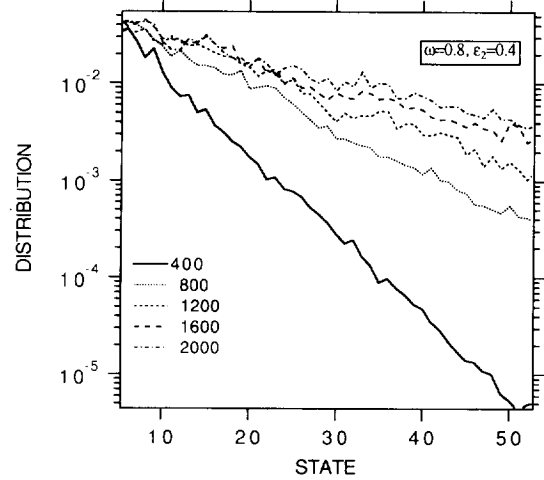


Fig. 3. Phonon distribution in the Fock space. The parameters are the same as in the case of $\epsilon_2 = 0.4$ in Fig. 2.

such a situation we may use the approximation (4) for the second mode, and the effect of the second mode can be well approximated by the time-dependent periodic perturbation with the frequency ω_2 . As shown in Fig. 2 ($\epsilon_2 = 0.1, 0.4$), the temporal behavior of the energy E_{el} , E_p and MSD in the dichromatic case is drastically different from the monochromatic one. It is evident that phonon energy exhibits a nice linear increase, while the electronic energy decreases monotonically until it reaches an almost zero energy level. We may judge that a one-way quasi-stationary energy flow from electron to phonons is realized until the electronic energy relaxes to a final state, and the flowing rate of energy increases in accordance with the increment in the coupling strength (β_1, β_2). The final electronic state with almost zero energy can be regarded as an equilibrium state extended over all the electronic energy eigenstates with even statistical weight.

Finally we focus our attention on the quantum statistical properties of phonon modes. Fig. 3 shows semi-log plots of the probability distribution in the Fock space of the first phonon mode measured at several time steps. The plots all compare with straight lines very well. Hence the distribution in the Fock space is the Boltzmann distribution

$$|\langle n | \Psi(t) \rangle|^2 \propto \exp[-n/k_B T(t)], \quad (7)$$

characterized by the time-dependent temperature $T(t)$ which rises as time elapses. The Boltzmann distri-

bution appears only when the linear growth of emitted phonon energy is observed. Thus the formation of the statistical distribution and the realization of irreversible energy transport must be both sides of the same stochastization phenomenon which is spontaneously induced within a closed quantum system itself without a coupling with any heat reservoir. It is surprising that such a nonequilibrium statistical behavior can be observed in a simple closed quantum system.

In conclusion, it has been demonstrated that an irreversible flow of energy from electron to phonons is induced spontaneously even though the number of phonon modes is only two. The electron scattered by an irregular potential emits its energy to the phonon modes, and moreover the phonons are excited to a thermal state characterized by a well-defined temperature. We emphasize here again the critical role of the irregularity in the scattering potential. In fact, if the scattering potential is periodic, it can be shown that both electronic energy and phononic energy oscillate around the initial energy level, and no net energy transfer is observed between electron and phonons. As has already been remarked, the origin of the irreversibility is the phase complexity peculiar to the localized eigenstates. Once the localization is dynamically destroyed by the perturbation of phonon modes, such a complexity in turn can cause the irreversible energy transfer to occur.

“Chaos” provides a promising mechanism which can create sufficient complexities to induce an apparently irreversible behavior in closed quantum systems [9]. However, as demonstrated in the present paper, spatial irregularity also plays a crucial role as an origin of quantum irreversibility when it is combined with a dynamical interference arising from other degrees of freedom. Such a mechanism will provide a simple dynamical modeling to understand the origin of resistivity in solid state materials. The next step of our study is to examine whether the electronic resistivity obeying Ohm’s law is described by the closed quantum model proposed here. Some progress is now being made, and the results will be presented elsewhere [17].

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