Electron-phonon interaction, localization, and polaron formation in one-dimensional systems

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We present results for the time evolution of a one-dimensional system consisting of an electron, described by a tight-binding Hamiltonian and a harmonic lattice, coupled by a deformation-type potential. We solve numerically the nonlinear system of equations of motion for this model in order to study the effects of varying the electronic effective mass for several initial conditions and coupling strengths. Different types of localized and extended states are formed with features that are absent from the traditional polaronic states and depend very strongly on the initial electronic configuration and effective mass in a very often unexpected manner. We find that, in general, an increase of the initial electronic energy decreases the ability of the system to form localized states. However, a large effective mass favors localized polaron formation for initially localized electrons, but this is not always the case for initially extended electronic states. In the latter case, increasing the effective mass of an electron initially close to the bottom of the band makes localization more difficult, while for an initially highly excited electron, localized polaron formation is possible only when the electronic effective mass and the atomic masses of the lattice become of the same order. Finally, for a small parameter range, we find an impressive recurrence, a periodic and a complete exchange between the electronic and vibrational degrees of freedom of a small part of the initial electronic energy.

I. INTRODUCTION

One of the fundamental problems in condensed matter physics is the interaction between electrons and lattice vibrations. Many basic properties of solids, such as electrical resistivity, depend on this interaction which is also responsible for processes such as superconductivity and polaron formation. A variety of different analytical approaches has been used to understand the behavior of electron-phonon systems, all of which involve certain approximations with commonly employed perturbative and adiabatic approaches. In the case of a single electron interacting with vibrational degrees of freedom, the general picture emerging from these studies is the electron self-trapping for sufficiently large electron-phonon coupling, i.e., the creation of an electronic state bound to the lattice distortion potential resulting from the presence of the electron. The polaron (the quasiparticle consisting of the electron and the induced lattice distortion) then moves as an entity in the crystal. The results depend on the approximations used which, in turn, depend on the parameter range under study. For instance, when the effective mass of the electron, m^*, is not large and the electron-phonon coupling α is small, a perturbation approximation in α results in a change of the electron effective mass by a factor of $(1\text{-}\frac{\alpha}{6})^{-1}$. As α increases, perturbation theory breaks down, predicting an enormous effective mass. Variational procedures and the method of canonical transformation that eliminates electron coordinates give an effective mass multiplied by $(1+\frac{\alpha}{6})$ for intermediate coupling.[1,2] In the case of a large effective mass (relevant to narrow-band materials) and strong coupling, the electron hopping energy between adjacent sites (J) is treated as a perturbation and the concept of the small polaron is introduced, i.e., of the electron localized at a few sites.[3] Even though many of these theories give some definitive and correct predictions, there are other very important aspects of the problem that are not successfully addressed, if addressed at all. Some very interesting regions of parameter space have not been fully explored due to the limitations of several approximations. The discovery of high-T_c superconductors has generated a new interest in narrow-band electron-phonon systems. There are several attempts to describe the intermediate regime.[4] Exact cluster solutions for different values of the adiabatic parameter and the coupling strength show that the adiabatic Holstein small polaron and the Lang-Firsov canonical transformation are in agreement with the exact solution in the adiabatic and nonadiabatic regimes, respectively.[5] However, a full description of the dynamics, i.e., the time evolution, of the electron-phonon systems is not possible within traditional methods, especially for highly excited states. Another interesting question is how disorder affects electron-phonon systems, especially near the phase transition point of propagating to localized eigenstates.[6] To answer some of these questions, a different approach has been developed in recent years. Over the last few decades, there has been an enormous activity in the relatively new field of nonlinear physics.

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A large number of systems in very different disciplines of physical sciences has been described by nonlinear models. The significant progress in nonlinear mathematics,[7–9] together with the development of computers which allow extensive numerical simulations, opens new possibilities in understanding nonlinear systems. Since nonlinearity, introduced by the coupling of the electron to the lattice, is present in electron-phonon systems, one expects to obtain some insight into the dynamics of the problem using nonlinear techniques. This approach has proved fruitful in the treatment of the interaction of an intramolecular excitation with the lattice vibrations in proteins[10,11] as well as the coupling of the latter to the off-diagonal electronic matrix element in polyacetylene.[12] Recently, some interesting numerical results of an electron propagating in a quasiperiodic one-dimensional model and interacting with lattice vibrations were presented.[13,14] Among other surprising findings, some strong deviations from the expected thermodynamic behavior were observed in the case of a highly excited electron. Indeed, it was found in Refs. 13 and 14 and was verified by the present work, that the traditional assumption that the electron gradually transfers its energy to the lattice within a few lattice times, reaches the bottom of the band, and the system reduces to a ground state problem, is not always correct. In fact, in most cases of highly excited electrons, long-lived metastable states have been reached, and for a small part of the parameter range, an impressive recurrence phenomenon was found.[15] In this paper, we present some of the results of a systematic numerical study of this electron-lattice system throughout the entire physically interesting parameter space. Special emphasis has been given to the effects of increasing the electronic effective mass. For certain parts of the parameter space, we found the behavior expected from approximate theories, but more often than not, our results show a richer, and sometimes unexpected behavior, especially in the range of parameters which is still unexplored or poorly understood. Apart from the rather obvious role of the electron-phonon coupling in the final outcome, we found that the final state reached by the system depends very strongly on the electron mass and the initial electronic state. One might naively think that "heavy" electrons are more localized than "light" electrons, but, as we will show here, this happens only for specific initial conditions, while for others, it is exactly the opposite situation or none of the above.

In Sec. II, we present our model, discuss the assumptions involved, and show how it relates to other existing models in some limiting cases. We also give an outline of our methods of calculation and a brief description of our numerical simulation. Section III consists of four subsections: in Sec. III A we present the results for the case of small electronic effective mass (adiabatic case), in Sec. III B for intermediate mass, in Sec. III C for large mass (nonadiabatic case), and in Sec. III D we give a simple interpretation of the results. Throughout Sec. IV, we elaborate on the antithermodynamic recurrent behavior found for a region of the parameter space and for certain initial conditions, and finally, in Sec. V, we conclude with a short summary of our results.

II. MODEL

The system under study is a one-dimensional, one-electron (i.e., our results are independent of particle statistics) model with the lattice vibrations being treated classically. More specifically, the Hamiltonian describing our system consists of an electronic part (H_e), a lattice part (H_ℓ), and the interaction part ($H_{e\text{-}l}$):

$$H = H_e + H_\ell + H_{e\text{-}\ell} \ . \tag{1}$$

The electronic part (H_e) is a tight-binding electron, with nearest neighbor interaction matrix elements ($-J$), i.e.,

$$H_e = \sum_n \epsilon_n |n\rangle\langle n| - J \sum_n |n\rangle(\langle n+1| + \langle n-1|) \ . \tag{2}$$

The diagonal matrix elements (ϵ_n) can be the same (periodic lattice) or different [e.g., $\epsilon_n = \epsilon_0 \cos(2\pi\sigma n)$, where σ is an irrational number, in the quasiperiodic case, or ϵ_n can be random numbers, in the disordered case]. During this work, they have been kept constant for all sites n ($\epsilon_n = 0$) in order to isolate the effects of electron-phonon coupling and the electron's effective mass without the complications arising from disorder. The results for a disordered system will be presented elsewhere. The local orbitals $|n\rangle$ are centered around the sites n ($n = 1, ..., N$) of the lattice with interatomic distance a. The eigenfunctions and eigenvalues of H_e are

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_n e^{ikna} |n\rangle \ , \tag{3a}$$

$$E_e = -2J \cos ka \ . \tag{3b}$$

The lattice part (H_ℓ) describes N coupled classical harmonic oscillators,

$$H_\ell = \frac{1}{2M} \sum_n p_n^2 + \frac{K}{2} \sum_n (u_{n+1} - u_n)^2 \ , \tag{4}$$

where $p_n = M\dot{u}_n$ and u_n are the momentum and the displacement of atom n, respectively, M is the atomic mass, and K is the spring constant between nearest neighbor atoms. H_ℓ supports acousticlike eigenvibrations with eigenfrequencies $\omega_q = \sqrt{\frac{4K}{M}} |\sin \frac{ka}{2}| \equiv 2\omega_0 |\sin \frac{ka}{2}|$ (the maximum frequency is $2\omega_0$ and the speed of sound is $c = \omega_0 a$). The consideration of acoustic vibrations in this one-dimensional model naturally leads to a deformation type of electron-phonon coupling, which is a short-range interaction and takes into account that the electron energy is affected by the strain produced by acoustic modes. Other models consider Fröhlich (polar) coupling or piezoelectric coupling. Deformation coupling occurs in all crystals and in our model it has the form

$$H_{e\text{-}\ell} = \chi \sum_n |n\rangle\langle n|(u_{n+1} - u_{n-1}) \ . \tag{5}$$

In Eq. (5), χ is the strength of the coupling and the deformation potential ($2a\chi$) is symmetrized.

Throughout our calculations, we use J, M, and $t_\ell \equiv \sqrt{M/K}$ as the natural units of energy, mass, and time, respectively. This choice leaves us with two parameters: (i) the adiabatic parameter $\hbar$, measured in units of $J\sqrt{M/K}$, or equivalently the dimensionless quantity $\frac{\hbar}{J\sqrt{\frac{M}{K}}} = \frac{\hbar/J}{\sqrt{\frac{M}{K}}} = \frac{t_e}{t_\ell}$, where $t_e = \hbar/J$ and t_ℓ are the characteristic electronic and lattice times, respectively; (ii) the coupling strength χ, measured in units of $\sqrt{JK}$, or equivalently the dimensionless quantity $\chi/\sqrt{JK}$ which is the square root of $\lambda = \frac{\chi^2}{KJ}$, similar to the one appearing in superconductivity. The unit of length a_0 is $\sqrt{J/K}$ in this natural system of units. The adiabatic parameter $\hbar = t_e/t_\ell$, i.e., the ratio of the characteristic electronic time over the lattice time, gives a measure of the effective mass of the electron relative to the lattice atoms mass. Thus, a small value of t_e/t_ℓ is relevant to the case where the electronic mass is small compared to the atomic masses ($t_e/t_\ell \simeq 0.01$ is typical for most metals). A large value of t_e/t_ℓ is relevant to a large electron mass (in very narrow-band materials the ratio t_e/t_ℓ may approach or even exceed unity). This becomes clear by writing

$$\frac{m^*}{M} = \frac{1}{2}\left(\frac{t_e}{t_\ell}\,\frac{a_0}{a}\right)^2 , \tag{6}$$

where $m^* = \hbar^2/2Ja^2$ is the electronic effective mass. A small value of m^*/M means that t_e/t_ℓ is small or that the lattice constant a/a_0 is large and a large m^*/M implies either a large t_e/t_ℓ or a small a/a_0. By varying t_e/t_ℓ from 0.01 to 10, we show how the changes of the electronic effective mass affect the behavior of the coupled electron-phonon system. The value of the coupling χ is varied between 0.2 and 4 (realistic values of $\lambda = \frac{\chi^2}{KJ}$ range from 0.1 to 1.7, for metals). Typical values for our natural units are $M = Am_u$, where A is the mass number and m_u is the atomic mass unit, and $K = 50\ N/m$, so that the unit of time is of the order $t_\ell \sim 10^{-15}$ sec.

The Hamiltonian (1) cannot be diagonalized exactly, and so there are two alternatives: Either use approximate theories suitable for each parameter regime or solve numerically the equations of motion that follow from (1). We choose the latter one in order to include all the different aspects of the problem.

The equations of motion for our system are derived from the Hamiltonian (1) with the electronic wave function written as $|\Psi_e(t)\rangle = \sum_n c_n(t)|n\rangle$. We should point out that we follow a semiclassical approach and we do not attempt a rigorous quantum mechanical treatment of the lattice vibrations. There is a significant amount of work related to the derivation of quantum mechanically consistent equations of motion for this type of Hamiltonian.[16–20] The main difficulty is that the ansatz states used for the electron-phonon system do not satisfy the Schrödinger equation, except for some special cases. In this work we simply write down the equations of motion for the electronic and the vibrational degrees of freedom and we examine the time evolution of this system of differential (in time) difference (in space) equations:

$$i\hbar\frac{\partial c_n}{\partial t} = \chi(u_{n+1} - u_{n-1})c_n - J(c_{n+1} + c_{n-1}) , \tag{7}$$

$$\frac{\partial p_n}{\partial t} = K(u_{n+1} + u_{n-1} - 2u_n) + \chi(|c_{n+1}|^2 - |c_{n-1}|^2) , \tag{8}$$

$$p_n = M\frac{\partial u_n}{\partial t}. \tag{9}$$

Our primary goal is to study the morphology of the solutions as a function of time. For this purpose, we examine the time dependence of the electronic amplitudes $c_n(t) = \langle n|\Psi_e(t)\rangle$, the lattice displacements $u_n(t)$, and the corresponding atomic velocities, $\dot{u}_n(t)$. In addition to the solutions, we monitor some meaningful quantities that provide very useful information about the system. These are the following.

(a) The electronic energy $[E_e(t)]$:

$$\begin{aligned} E_e(t) &= \langle\Psi_e(t)|H_e|\Psi_e(t)\rangle \\ &= -J\sum_n c_n^\dagger(t)[c_{n-1}(t) + c_{n-1}(t)]. \end{aligned} \tag{10}$$

(b) The lattice energy $[E_\ell(t)]$:

$$E_\ell(t) = \frac{M}{2}\sum_n \dot{u}_n^2(t) + \frac{K}{2}[u_{n+1}(t) - u_n(t)]^2. \tag{11}$$

(c) The interaction energy $[E_{e\text{-}\ell}(t)]$:

$$E_{e\text{-}\ell}(t) = \chi\sum_n c_n^\dagger(t)c_n(t)[u_{n+1}(t) - u_{n-1}(t)]. \tag{12}$$

(d) The participation number $[P(t)]$:

$$P(t) = \left[\sum_n |c_n(t)|^4\right]^{-1}. \tag{13}$$

The quantity P is very convenient in characterizing the electronic wave function. Its value gives a measure of how many sites participate in the wave function at a given instance. It takes values ranging from $P = 1$ (when the electron is localized at a single site) to $P = N$ (when the electronic wave function is uniformly extended over the whole length of the specimen).

The numerical solution of Eqs. (7)–(9) for relatively large times and atomic chains requires heavy computation. In order to obtain a realistic picture for the system, it is necessary to run simulations for hundreds of atoms and thousands of characteristic lattice times (t_ℓ). Typical runs include $N = 300$–600 atoms and times of the order of $10^4 t_\ell$ or $10^5 t_\ell$. It is also necessary to cover a large portion of the parameter and initial condition space. For these reasons the use of parallel computers becomes imperative (almost all of the simulations were performed on nCube machines). For the time integration, we use a fourth-order Runge-Kutta method with a step equal to $10^{-4}t_\ell$ or $10^{-3}t_\ell$ (with this step size, energy is conserved with a relative accuracy of at least 10^{-5}). Throughout

the simulations, periodic boundary conditions are used ($c_{N+1} = c_1$, $u_{N+1} = u_1$). Initially the lattice is at rest and undeformed (i.e., we restrict ourselves to the zero-temperature case), while the electron is either localized at a single site or placed very close to an eigenstate (3) with energies $E_e \simeq -2, -1$, and 0.

After describing our model, it is interesting to point out some of its limiting behaviors. An approximation quite often used in electron-phonon systems is the so-called adiabatic approximation.[21] When the lattice atomic mass (M) is much larger than the electron's effective mass (m^*) the motion of the electron is very rapid compared to the motion of the lattice. It is possible then to attribute an infinite mass to the atoms (or a zero phonon frequency) and consider a very heavy lattice that cannot follow the instantaneous electronic motion but responds to the probability that the electron is in a particular site. This practically translates to the fact that the kinetic energy of the lattice can be safely neglected from the Hamiltonian (1); then, following Holstein's treatment of the large polaron,[22], by minimizing the energy with respect to the u_n's, it is straightforward to derive the following discrete nonlinear Schrödinger (DNLS) equation:

$$\left[\frac{\chi^2}{K}(|c_{n+1}|^2 + |c_{n-1}|^2 + 2|c_n|^2) - \varepsilon\right] c_n + J(c_{n+1} + c_{n-1}) = 0 \ , \quad (14)$$

with $u_{n+1} - u_n = -\frac{\chi}{K}(|c_n|^2 + |c_{n+1}|^2)$, $-\varepsilon = E - \frac{K}{2}\sum_\ell (u_{\ell+1} - u_\ell)^2$. For the case of a large polaron where the characteristic length far exceeds the lattice constant a, the continuum approximation is justified and it gives the continuous nonlinear Schrödinger (NLS) equation

$$\left(\frac{4\chi^2}{K}|c_n|^2 - \varepsilon + 2J\right) c_n + J\frac{\partial^2 c_n}{\partial n^2} = 0. \quad (15)$$

One solution of Eq. (15), for electronic states decaying at infinity and for the normalization condition $\int c_n^2 dn = 1$, is

$$c_n = \left(\frac{\chi^2}{2KJ}\right)^{1/2} \mathrm{sech}\left[\frac{\chi^2}{KJ}(n - n_0)\right], \qquad \varepsilon = 2J + \frac{\chi^4}{K^2 J}. \quad (16)$$

The result (16) describes a self-trapped solution of Eq. (15) with the energy of the localized electron ($-\varepsilon$) lowered by χ^4/K^2J relative to the corresponding ground state energy $-2J$ of the delocalized Bloch electron of (3). In addition to the solution (16), Eq. (15) possesses two other hierarchies of solutions, i.e., Bloch-like solutions and other periodic solutions given by Jacobian elliptic functions.[23]

The time-dependent DNLS equation corresponding to (14) is

$$i\hbar\frac{\partial c_n}{\partial t} + \frac{\chi^2}{K}(|c_{n+1}|^2 + |c_{n-1}|^2 + 2|c_n|^2)c_n + J(c_{n+1} + c_{n-1}) = 0. \quad (17)$$

Equation (17) can also be obtained from Eqs. (7)–(9) under certain assumptions by letting $\frac{\partial p_n}{\partial t} \simeq 0 \Leftrightarrow M\frac{\partial^2 u_n}{\partial t^2} \simeq 0$, which is the adiabatic limit when $\frac{\partial^2 u_n}{\partial t^2} \simeq 0$ or the, sometimes called, antiadiabatic limit when $M \simeq 0$. The latter becomes physically meaningful in the case of large ω_q, when the lattice modes can follow instantaneously the motion of the electron (sometimes the lattice is said, rather confusingly, to follow the electron motion adiabatically).

Within the continuous limit, Eq. (17) reduces to the time-dependent continuous nonlinear Schrödinger (NLS) equation which admits three branches of solutions: soliton (self-trapped) solutions, Bloch-like solutions, and the so-called "cnoidal wave" solutions, which are periodic in space and time, propagating type of solutions.[10] The choice of the solution by the system depends on the initial condition. The properties of the NLS equation and its several discretizations have been studied extensively since the NLS equation appears in many different problems of several branches of physics, such as plasma physics, nonlinear optics, Ginzburg-Landau theory of superconductivity, magnetic chains, and also in fluid mechanics, biology (Davydov solitons), electrical networks, etc. Obviously the NLS equation is very important in its own right but one must keep in mind that in coupled electron-phonon systems it is only an approximate description of the system in the adiabatic and continuous limit. Our model exhibits a much richer behavior as expected due to the full consideration of the lattice vibrations in a wide range of parameters. It is a more realistic description of the electron-phonon interaction problem and since it is nonintegrable, in general, it possesses dynamical properties that are absent from the integrable NLS equation[24] or, for that matter, from some integrable DNLS equations.[25–27] Our results fully include the effects of lattice vibrations, discreteness, dispersion, and nonlinearity (and, potentially, of disorder) in the whole range of parameters (from the adiabatic to the antiadiabatic and from the weak to the strong coupling regime) and initial conditions.

III. RESULTS AND DISCUSSION

We studied the problem for different values of t_e/t_ℓ, of the electron-phonon coupling (χ), of the size of the chain (N), and for several initial conditions. The polarons can be classified according to the final state of the system in three broad classes:[14] (a) extended (E) states characterized by an electronic wave function that extends over all sites without a pronounced peak, a large participation number ($P \geq N/3$), and a small value of $|E_{e\text{-}l}|$ in comparison with E_ℓ; (b) localized (L) or self-trapped polarons characterized by an electronic wave function that has one or more pronounced peaks and decays away from them, and a small participation number ($P \leq N/5$); (c) intermediate (I) polarons characterized by a wave function that has one or more peaks but does not seem to decay away from them and a participation number that ranges between $N/5$ and $N/3$.

Since in this work we are interested in studying how

the electron-lattice system behaves when the electronic mass changes, we present results for different values of t_e/t_ℓ.

A. Small electron mass ($t_e/t_\ell \simeq 0.01$)

The value of the ratio of the electronic time over the lattice time $t_e/t_\ell = 0.01224$ is typical for most metals and this case has been studied extensively in Refs. 13 and 14. Our results confirm the behavior already observed and, in addition, they reveal some remarkable features of the system. More specifically, for a narrow region of the initial condition and the parameter space a small fraction of the electronic energy is transferred to the lattice and then completely back to the electron with an impressive regularity[15] (see, also Sec. IV). Some of the results presented in this subsection are similar to the ones already discussed in Ref. 14 in order to focus attention on some features which are strongly modified as the electronic time t_e becomes comparable to the lattice vibration time t_ℓ.

When the initial energy of the electron is close to the bottom of the band [$E_e(0) \simeq -2$] we recover the expected ground state behavior for a one-dimensional (1D) system; i.e., a polaron is formed even for weak coupling ($\chi \geq 0.2$). Such a polaron is shown in Fig. 1, for $\chi = 0.308$, $N = 300$, $t_e/t_\ell = 0.01224$, and the electron being initially very close to the eigenstate of H_e with $E_e = -2$ (ground state with $c_n = 1/\sqrt{N}$). The shape of the localized electronic wave function, Fig. 1(a), is approximately the soliton type obtained analytically within the adiabatic approximation, Eq. (16). The participation number P is approximately 35 with relatively small fluctuations [Fig. 1(e)]. The polaron formation is accompanied by an increase in the electronic energy [$\delta E_e \equiv E_e(t) - E_e(0) \simeq 0.003$, Fig. 1(d)] due to the confinement (the electron energy being purely kinetic). The lattice energy [Fig. 1(b)] increases from zero to $E_\ell = 0.006$ and the interaction energy [Fig. 1(c)] becomes $E_{e\text{-}\ell} = -0.009$. By increasing the electron-phonon coupling, the process of polaron formation becomes faster, the spatial extent of the polaron

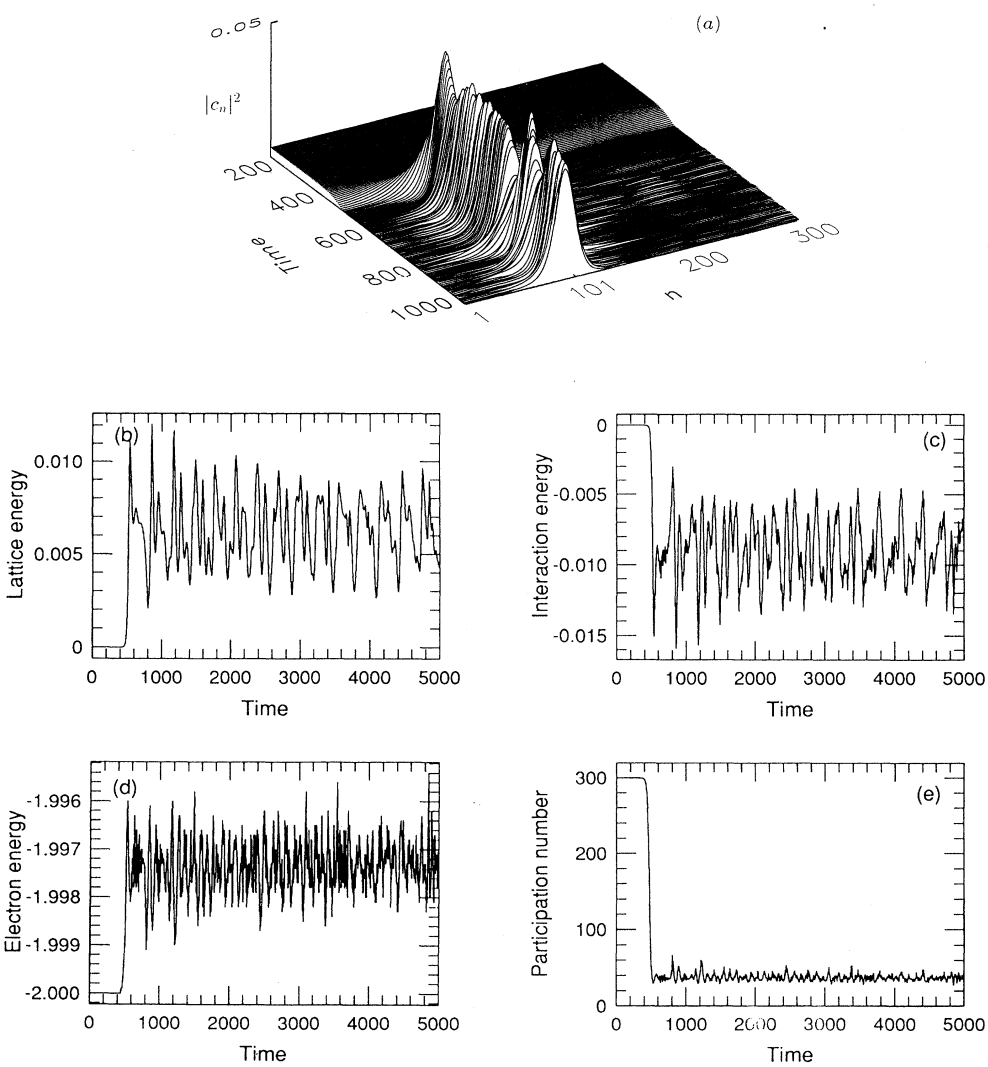

FIG. 1. Localized polaron formation for a system with $N = 300$, $t_e/t_\ell = 0.01224$, $\chi = 0.308$ (weak coupling), and initial electronic state with $E_e(0) \simeq -2$. The unit of time is t_ℓ and of energy is J. The time evolution of the electronic wave function $|c_n(t)|^2$ (a), the lattice energy (b), the interaction energy (c), the electronic energy (d), and the participation number (e) are shown.

becomes smaller, and the changes to the initial energies $[E_e(0), E_\ell(0), E_{e\text{-}\ell}(0)]$ much more significant (for $\chi \approx 2$, $|E_\ell|$ and $|E_{e\text{-}l}|$ can take values of the order of 1). The kinetic energy of the lattice cannot be neglected and the adiabatic approximation cannot be used. This transition from the large polaron in the weak coupling region to the small polaron in the strong coupling region is the typical behavior in the adiabatic limit.

A similar picture emerges for the low-lying excited states but this changes completely as the initial electronic energy gets considerably higher: It becomes impossible to obtain localized polarons unless the value of the coupling χ reaches very high and unrealistic values. According to the expected behavior of a highly excited electron, polaron formation should become possible after a gradual transfer of the electronic energy to the lattice (within a few lattice times t_ℓ) until the electron reaches the ground state. But what happens instead is that this transfer of energy slows down and eventually it seems to stop (on the average) without the electron being thermally equalized with the lattice. This seemingly antithermodynamic behavior is, in most cases, associated with a very complicated, almost chaotic time evolution. However, for the excited state close to $E_e(0) = -1$ and for a small part of parameter space, we found a very regular behavior: The electron initially placed close to this highly excited eigenstate, after transferring a small fraction of its energy to the lattice, absorbs back the transferred energy and the system returns to its initial state. We will elaborate on this remarkable recurrence phenomenon in Sec. IV. For the excited electronic states with $E_e(0) \simeq -1$ and for weak coupling, the electron hardly interacts with the lattice. For a relatively small range of the coupling strength ($1.35 < \chi < 1.57$) the recurrent behavior is observed and for strong coupling ($\chi \simeq 2$) the system is driven to an intermediate state. Such an intermediate state is shown in Fig. 2. The value of the coupling constant is $\chi = 2$ and, as in the case of Fig. 1, $N = 300$, $t_e/t_\ell = 0.01224$. The electron initially placed close to the eigenstate with $E_e(0) = -1$ transfers most of its energy to the lattice and reaches close to the bottom of the band [Fig. 2(d)]. However, the interaction energy [$E_{e\text{-}\ell} \sim 0.1$, Fig. 2(c)]

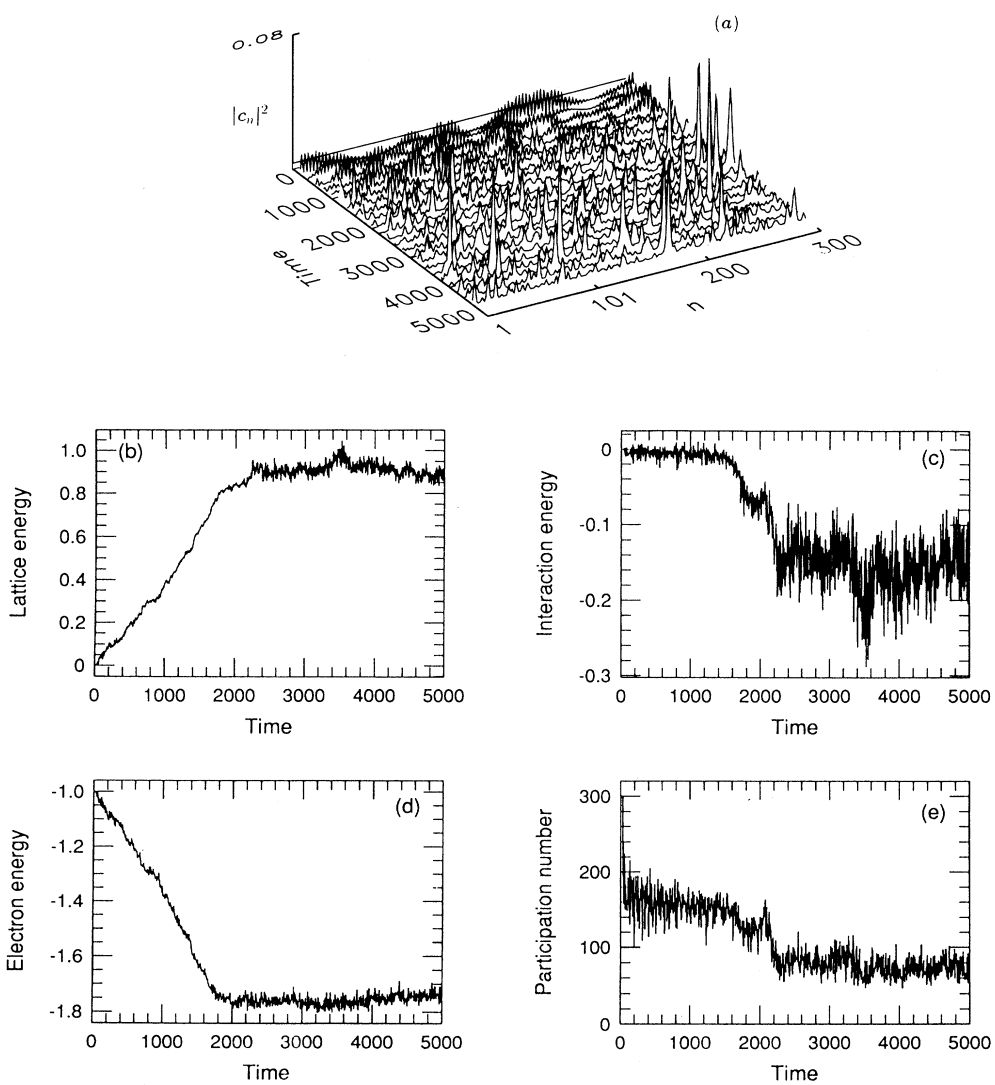

FIG. 2. Intermediate state for a system with $N = 300$, $t_e/t_\ell = 0.01224$, $\chi = 2$ (strong coupling), and initial electronic state with $E_e(0) \simeq -1$. The unit of time is t_ℓ and of energy is J. The time evolution of the electronic wave function $|c_n(t)|^2$ (a), the lattice energy (b), the interaction energy (c), the electronic energy (d), and the participation number (e) are shown.

remains very small relative to the lattice energy [$E_\ell \sim 1$, Fig. 2(b)] and the electronic wave function [Fig. 2(a)] is not really localized. The result is an intermediate state reached at $t \simeq 2000t_\ell$. For even larger values of the coupling constant ($\chi \geq 2.5$) the final state is a localized polaron.

As the energy of the initial electronic state further increases, the electron-lattice interaction energy becomes smaller, even for very strong coupling. For instance, when $E_e(0) \simeq 0$, the system practically remains in its initial extended state for any realistic value of the coupling strength.

In all the cases mentioned so far, the electron was initially placed very close to an eigenstate of H_e. In Fig. 3, we show the time evolution of the system when the electron is initially confined to a single site [$E_e(0) = 0$], with $\chi = 2$, $t_e/t_\ell = 0.01224$, $N = 377$. After $t = 5000t_\ell$ a steady state has not been reached yet. The electron, after spreading across the specimen in a short time (of the order of t_ℓ), transfers little of its energy to the lattice at a slow rate. The interaction energy remains close to zero and the participation number fluctuates around $P \simeq 190$. There is no indication of localization and the system is clearly in an extended state.

In general, in the adiabatic case, i.e., when the electronic effective mass is small, the behavior of the system can be briefly described as follows.

Depending on the energy and the electron-phonon coupling, the system reaches an extended, localized, or intermediate state. For any initial state, it is apparent that increasing χ favors the confinement of the electron. Whether or not self-trapping of the electron will occur depends on the initial state: It happens easily (even for very weak coupling) for the initial state being the ground or a low excited state and it gets harder as the initial energies get higher, becoming impossible for any realistic value of the coupling constant χ close to the center of the band. This picture is in agreement with Ref. 14 and quite different from the conventional one.

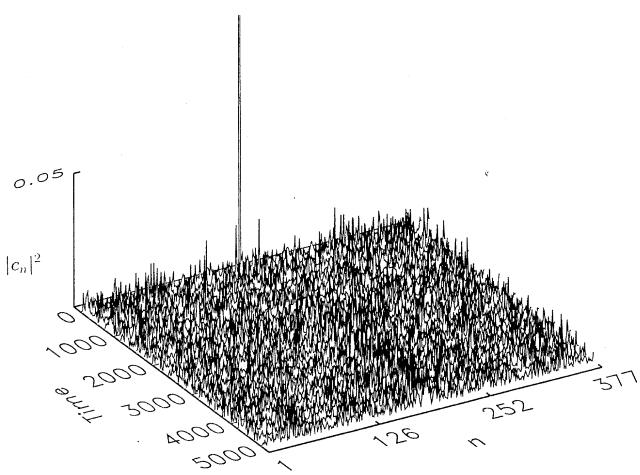

FIG. 3. The time evolution of the electronic wave function $|c_n(t)|^2$ in the case of an extended state for a system with $N = 377$, $t_e/t_\ell = 0.01224$, $\chi = 2$ (strong coupling), and initial electronic state localized at a single site [$E_e(0) = 0$]. The unit of time is t_ℓ.

B. Intermediate electron mass ($t_e/t_\ell \simeq 0.1$)

Increasing the ratio t_e/t_ℓ by a factor of 10 does not change the behavior of the system dramatically but the picture becomes different from the case of the small electron mass of Sec. III A. As in Sec. III A, when the electron is initially at the bottom of the band [$E_e(0) = -2$] or at a low-lying excited state, a weak coupling is sufficient for the creation of localized polarons. As the initial electronic energy increases, a larger coupling is required in order to obtain localized states. The main difference between the intermediate mass and the small mass cases is the possibility of localized states for highly excited (at the center of the band) intermediate mass electrons, as opposed to the small mass electrons considered earlier. But the values of the coupling strength necessary in order to obtain localized polarons still remain very high. When $E_e(0) \simeq -1$, localized states appear for $\chi \geq 2$. At the center of the band, i.e., $E_e(0) \simeq 0$, a very large value of $\chi \geq 3$ is required. An example is shown in Fig. 4. The initial electronic energy is $E_e(0) = -0.008\,333\,1$ and $\chi = 3$, $N = 377$, $t_e/t_\ell = 0.1$ [here, instead of starting with an almost eigenstate (3a), i.e., $c_n = \frac{1}{\sqrt{N}}e^{ikna}$, the imaginary part of $c_n(0)$ is taken to be zero; the initial condition (3a) gives a very similar behavior]. The electron transfers a significant amount of energy [Fig. 4(d)] to the lattice [Fig. 4(b)] and interaction [Fig. 4(c)] energies, without reaching the bottom of the band, and the participation number [Fig. 4(e)] drops to about $P \simeq 50$, as opposed to the corresponding case with $t_e/t_\ell = 0.01224$, where the system just stays in the initial state.

If an intermediate mass electron is initially localized at a single site, the final state is localized if $\chi \geq 3.5$ and the energy transferred is larger than the small mass case.

C. Large electron mass ($t_e/t_\ell \geq 1$)

The case where the effective mass of the electron becomes of the order of the atomic mass is relevant to narrow-band materials and presents substantial differences from the small electron mass case of Sec. III A. The process of localized polaron formation when the electron is close to or at the bottom of the band initially [$E_e(0) \simeq -2$] becomes slower (more than the expected two orders of magnitude due to the increase of t_e) and a weak coupling ($\chi < 1$) seems to be inadequate for self-trapping. In Fig. 5, the electron is initially at $E_e(0) \simeq -2$ and $N = 377$, $\chi = 1.5$, $t_e/t_\ell = 1$. The localized polaron formation is not fast and abrupt but instead there are relatively smooth fluctuations around an intermediate state [Fig. 5(a)] before the electron becomes localized through a steplike process after $t \simeq 3800t_\ell$ [Figs. 5(b)–5(e)] and the participation number drops to $P \simeq 20$ [Fig. 5(e)]. When t_e/t_ℓ becomes extremely high ($t_e/t_\ell \sim 10$), the process becomes even slower and requires unrealistically large coupling ($\chi > 3$).

When an electron with $t_e/t_\ell \simeq 1$ is initially in higher-energy states, localization is more difficult than the ground state, but it is remarkably easier compared with the corresponding small mass electron case, where it was impossible for any realistic value of the coupling strength. More specifically, when $t_e/t_\ell \simeq 1, 2$ and the electron is excited close to an eigenstate with $E_e(0) \simeq -1$, a localized final state is reached if $\chi \geq 1.5, 1$, respectively. When $t_e/t_\ell \sim 10$ and $1.5 \leq \chi \leq 2.5$, the system undergoes a transition to an intermediate state with some of the electronic energy (E_e) transferred to the lattice (E_ℓ) and then returns to an extended state with $E_e \simeq -1$ and $E_e \simeq E_{e\text{-}l} \simeq 0$ while for $\chi \geq 3$ the final state is localized. In the case of $E_e(0) \simeq 0$, localized states are achieved for $t_e/t_\ell \sim 1$ and $\chi \geq 2.5$ (strong coupling) while for $t_e/t_\ell \simeq 10$ the result is an extended state for any coupling strength.

A very different behavior between the cases $t_e/t_\ell \geq 1$ and $t_e/t_\ell \simeq 0.01$ is also observed when the electron is initially confined to a single site [$E_e(0) = 0$]. The heavy electrons in this case end up localized for strong coupling ($\chi \geq 2$ for $t_e/t_\ell \sim 1$). In fact, the heavier the electron (i.e., the larger t_e/t_ℓ), the smaller the coupling required for self-trapping. In Fig. 6, an electron with $t_e/t_\ell = 1$, initially localized at a single site, and interacting with the lattice with $\chi = 2$, remains localized at a few neighboring sites. The electronic wave function [Fig. 6(a)] does not spread across the chain (as in the corresponding case of Fig. 3 with $t_e/t_\ell = 0.012\,24$) and the participation number [Fig. 6(e)] remains close to $P \simeq 12$. There is a significant transfer of energy from the excited electron at the center of the band to the lattice [Fig. 6(b)] and to the interaction [Fig. 6(c)] energy but the electron does not reach the bottom of the band; instead, it stays at $E_e \simeq -1$ [Fig. 6(d)]. A similar situation with $t_e/t_\ell = 2$ and $\chi = 1.0$ is shown in Fig. 7, but in this case the coupling is not strong enough and the localized state is relatively short lived (at $t = 5000t_l$, shown in the figure, the participation number is already $P \simeq 50$ and it further increases with time, reaching $P \simeq 190$ when

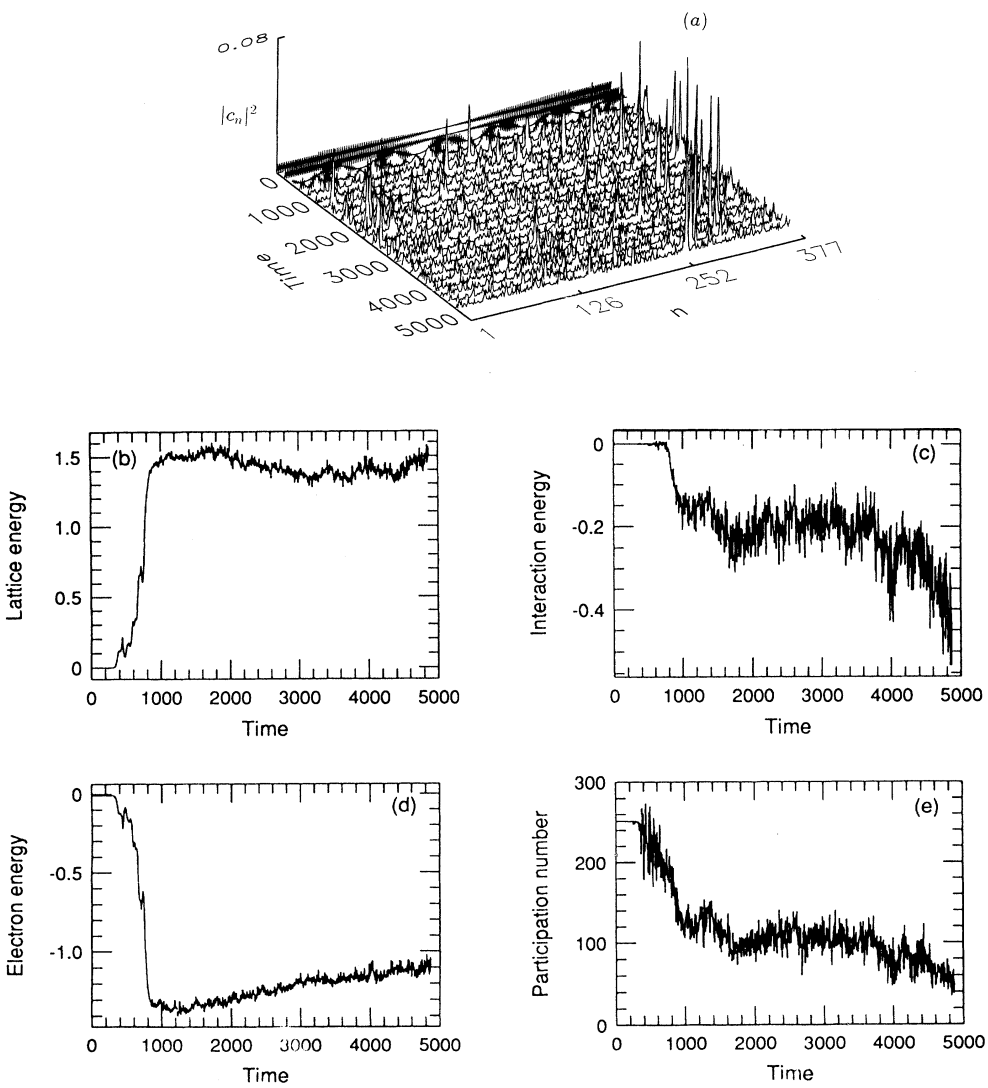

FIG. 4. Localized state for a system with $N = 377$, $t_e/t_\ell = 0.1$, $\chi = 3$ (very strong coupling), and initial electronic state with $E_e(0) \simeq -0.0083331$. The unit of time is t_ℓ and of energy is J. The time evolution of the electronic wave function $|c_n(t)|^2$ (a), the lattice energy (b), the interaction energy (c), the electronic energy (d), and the participation number (e) are shown.

the system reaches a steady state, not shown here). In Fig. 8, $t_e/t_\ell = 10$, $\chi = 2$, and the extremely heavy electron essentially is trapped by the two neighboring sites only with P between 1 and 2. The lattice energy becomes extremely high ($E_e \simeq 7$) in a very short time and so does the interaction energy ($E_{e\text{-}\ell} \simeq -6$). The electron energy fluctuates around $E_e \simeq -1$ and the electron remains in this excited localized state without reaching $E_e \simeq -2$ (bottom of the band). This situation, shown in Fig. 8, might not describe a realistic system due to the extremely large value of t_e/t_ℓ, but it exhibits dramatically the effects of increasing the electronic effective mass.

D. Interpretation of the results

The general picture that emerges from our results about the polaronic states formed in this coupled electron-lattice system for several initial electronic states, effective masses, and coupling strengths is summarized in Fig. 9: Figure 9(a) corresponds to the case with the electron initially placed close to the eigenstate with $E_e = -2$ (ground state), Fig. 9(b) to $E_e \simeq -1$, Fig. 9(c) to $E_e \simeq 0$, and Fig. 9(d) to the case where the electron is initially localized at a single site. For every case, on the χ versus t_e/t_ℓ plane, localized final states are indicated by solid circles and extended states by open circles (some intermediate states are also shown). These "phase" diagrams describe the state reached after a time of the order of $10^5 t_\ell$.

A rather intuitively obvious property of our model is that increasing the electron-lattice coupling favors localization in any case.

The final state of the system depends strongly on the initial electronic state. When the electron is initially very close to an eigenstate, the ability to form a localized polaronic state decreases as one moves from an initial state at the bottom of the band [$E_e(0) = -2$] to the center of the band [$E_e(0) = 0$], regardless of the electronic mass [Figs. 9(a)–9(c)] with the exception of $t_e/t_\ell \simeq 10$, where the value of the coupling required for localized polarons

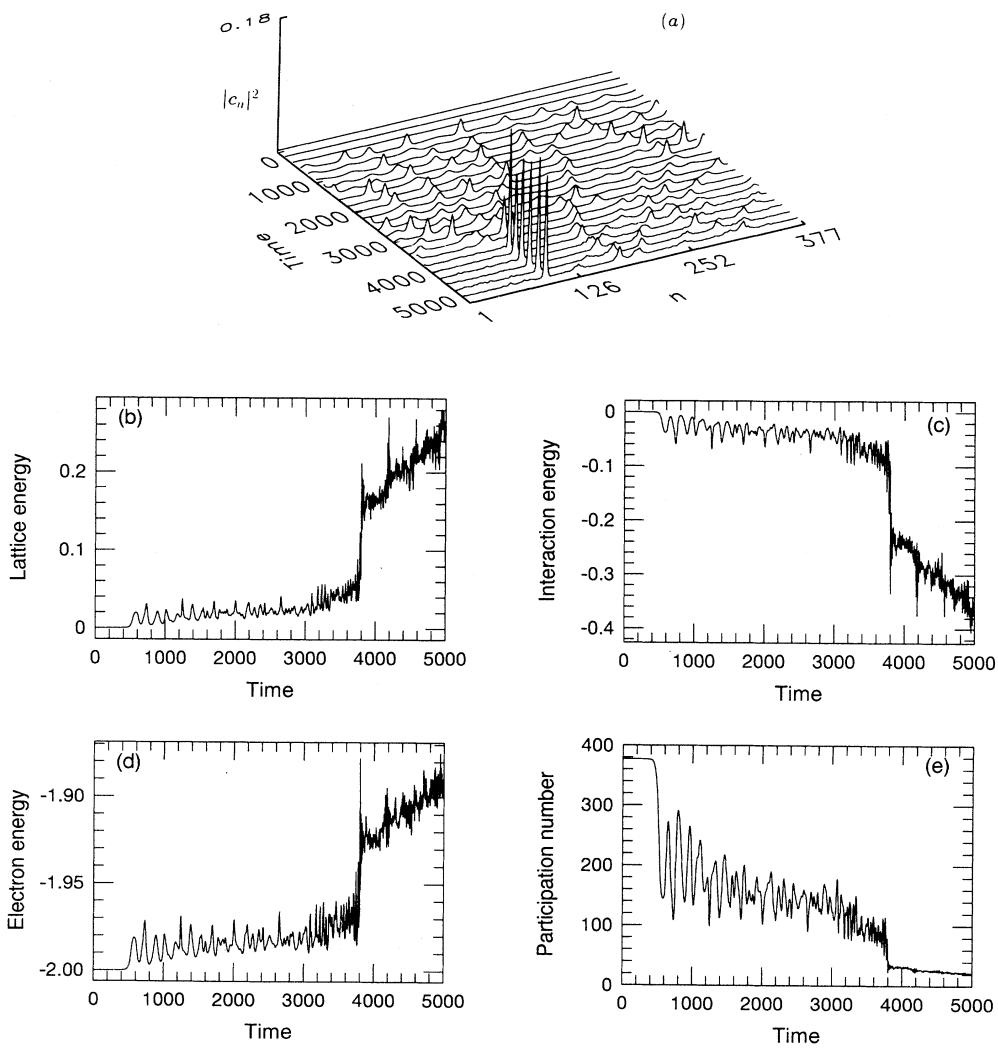

FIG. 5. Localized state for a system with $N = 377$, $t_e/t_\ell = 1$, $\chi = 1.5$, and initial electronic state with $E_e(0) \simeq -2$. The unit of time is t_ℓ and of energy is J. The time evolution of the electronic wave function $|c_n(t)|^2$ (a), the lattice energy (b), the interaction energy (c), the electronic energy (d), and the participation number (e) are shown.

becomes slightly smaller as one goes from the ground state to $E_e(0) \simeq -1$ [Figs. 9(a), 9(b)]. For initially highly excited states, we observe an "antithermodynamic" behavior in the sense that the electron does not transfer all of its energy and does not reach the bottom of the band in most cases. Metastable states have been found. The effects of changing the electronic effective mass are very profound. At the bottom of the band, increasing the mass does not favor localized polaron formation [Fig. 9(a)]. On the contrary, when the electron is initially highly excited, polaron formation becomes easier when the electronic and atomic masses become of the same order [Figs. 9(b),9(c)]. But further increase of t_e/t_ℓ results in extended final states. Although one might expect that the heavier the electron, the easier to localize, our results indicate that this is not the case when the electron is initially close to an eigenstate. This argument is valid if the electron is initially placed at a single site: The final state is extended for small electron mass and localized for large electron mass and sufficiently strong coupling [Fig. 9(d)].

In order to understand the behavior summarized above, we can resort to some simple qualitative arguments. The initial electronic states we consider are either localized in k space [very close to the eigenstates (3a) of H_e with energies (3b)] or localized in real space at a single site. The self-trapping mechanism is quite different in these two cases. In the former case, one electronic mode interacts with the vibrational modes of the lattice. This interaction is most efficient when the velocities of the electron and the lattice vibrations are the same, i.e.,

$$v_e \sim v_\ell. \tag{18}$$

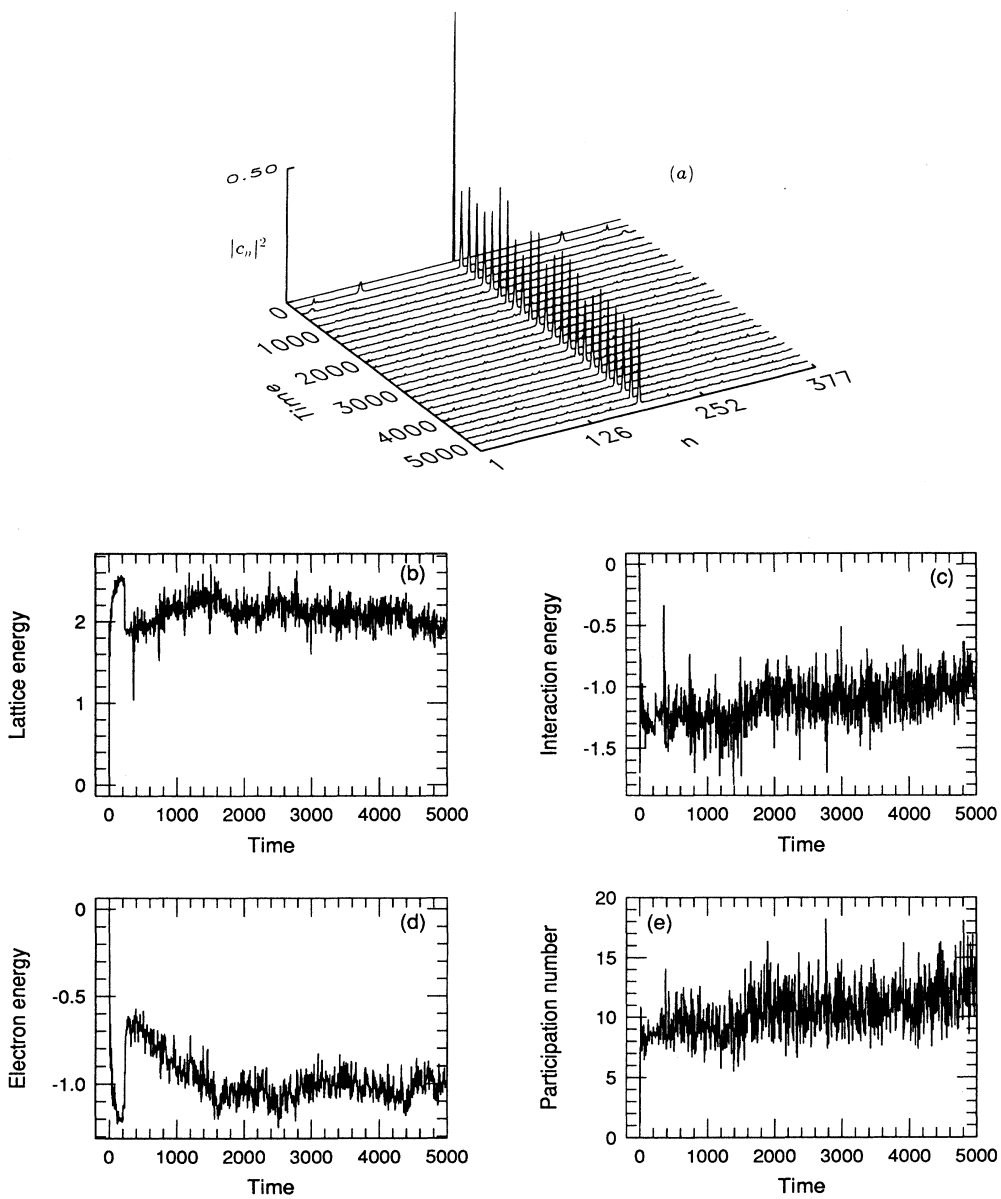

FIG. 6. Localized state for a system with $N = 377$, $t_e/t_\ell = 1$, $\chi = 2$ (strong coupling), and initial electronic state localized at a single site [$E_e(0) = 0$]. The unit of time is t_ℓ and of energy is J. The time evolution of the electronic wave function $|c_n(t)|^2$ (a), the lattice energy (b), the interaction energy (c), the electronic energy (d), and the participation number (e) are shown.

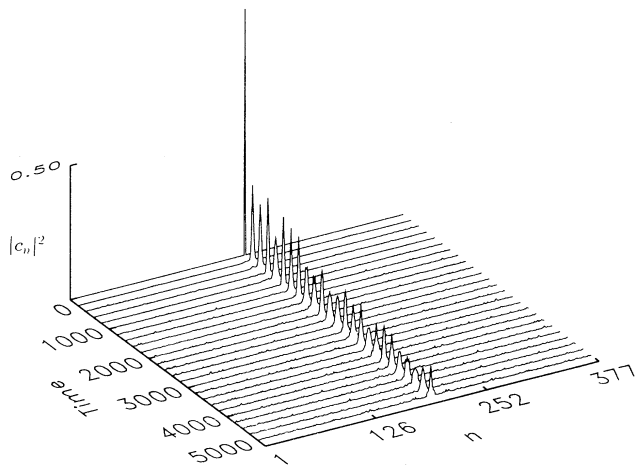

FIG. 7. Initially localized state that becomes extended for a system with $N = 377$, $t_e/t_\ell = 2$, $\chi = 1$ (intermediate coupling), and initial electronic state localized at a single site $[E_e(0) = 0]$. The unit of time is t_ℓ. The time evolution of the electronic wave function $|c_n(t)|^2$ is shown.

The group velocity of the electron is

$$v_e = \frac{1}{\hbar}\frac{dE_e}{dk} = \frac{2Ja}{\hbar}\sin ka = \frac{a}{\hbar}\sqrt{4J^2 - E_e^2}. \tag{19}$$

Since the lattice is initially undistorted, the average speed of its vibrations is

$$v_\ell \simeq c = a\sqrt{\frac{K}{M}}. \tag{20}$$

This assumption is valid in most cases since, except for very few situations, all the lattice modes are excited by the interaction with the electron. The condition (18), together with (19) and (20), gives in our units

$$v_e \simeq v_\ell \Rightarrow (4 - E_e^2)^{1/2} \simeq \hbar = \frac{t_e}{t_\ell}. \tag{21}$$

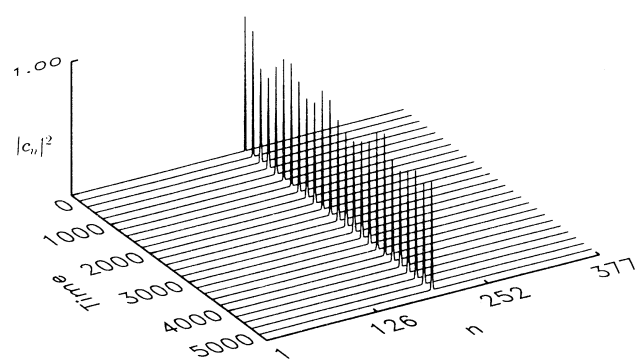

FIG. 8. Localized state for a system with $N = 377$, $t_e/t_\ell = 10$, $\chi = 2$ (strong coupling), and initial electronic state localized at a single site $[E_e(0) = 0]$. The unit of time is t_ℓ. The time evolution of the electronic wave function $|c_n(t)|^2$ is shown.

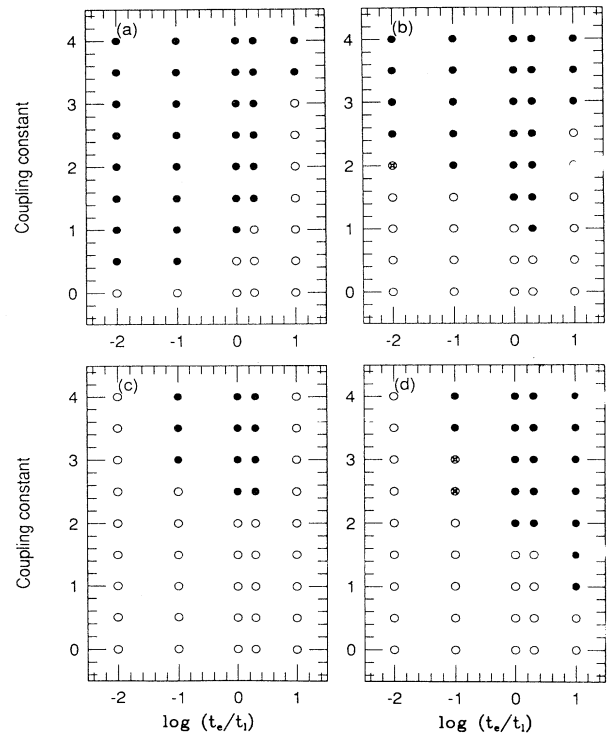

FIG. 9. The (χ)-(t_e/t_ℓ) parameter space for several initial conditions. On the horizontal axis the logarithm of the ratio t_e/t_ℓ is taken and on the vertical it is the coupling strength χ. In (a) the initial electronic state is very close to the eigenstate of H_e with $E_e(0) = -2$, in (b) to the one with $E_e(0) = -1$, in (c) to the one with $E_e(0) = 0$, and in (d) the electron is initially localized at a single site. The open circles indicate extended states and the solid ones localized states, while the intermediate states are shown with the crossed circles. These states were reached after real time simulations of $10^5 t_\ell$.

For $E_e(0) = -2$, condition (21) is satisfied for $t_e/t_\ell \to 0$. In other words, the electron-lattice interaction that results in electron self-trapping and polaron formation is more efficient for small electron mass and this is indeed what we found [Fig. 9(a)]. For $E_e(0) = -1$ and $E_e(0) = 0$, condition (21) gives $t_e/t_\ell \simeq 1.73$ and $t_e/t_\ell \simeq 2$, respectively. This is in agreement with our result that for highly excited states, self-trapping occurs more easily (for reasonable values of the coupling) when t_e/t_ℓ is 1 and 2 [Figs. 9(b),9(c)]. In the case of $t_e/t_\ell \simeq 0.01$, as well as $t_e/t_\ell \simeq 10$, at the center of the band, localized polaron formation does not take place for any realistic value of the coupling constant [Fig. 9(c)].

In the case of an electron initially localized at a single site the initial state is a superposition of different eigenstates (3a). Many electronic modes interact with the lattice so that once the electronic wave function is spread across the chain there is no mechanism such as the "resonance"-type condition (18) to confine the electron. Due to its energy, the "fast" electron ($t_e/t_\ell \simeq 0.01$) resists self-trapping, and due to the difference in t_e and t_ℓ, the "slow" lattice cannot respond before the electron

extends all over the specimen. But when t_e and t_ℓ become the same (or when $t_e \geq t_\ell \Leftrightarrow t_e/t_\ell \geq 1$) the lattice sites close to the electron can follow instantaneously the motion of the electron and the interaction can result in electron confinement, provided it is strong enough. The question of how strong can be answered using the Holstein small polaron formation criterion[3] which can be derived by considering the electron interacting with only its two neighboring sites:

$$\frac{\chi^2}{KJ} > \frac{J}{\hbar\omega_0} \tag{22}$$

or, in our units, $\chi^2 > 1/\hbar = t_\ell/t_e$. Condition (22) shows that the electron-phonon coupling λ has to be larger than the ratio of the order of the bandwidth (J) over the phonon energy ($\hbar\omega_0$), which can be the case in narrow-band materials. For $t_e/t_\ell = 0.01, 0.1, 1, 2, 10$, we find $\chi > 10, 3.16, 1, 0.71, 0.32$, respectively, in qualitative agreement with our results [Fig. 9(d)].

IV. RECURRENCE

The remarkable recurrence phenomenon,[15] which is reminiscent of the Fermi-Pasta-Ulam results,[28] is shown in Fig. 10, with $t_e/t_\ell = 0.01224$, $\chi = 1.5$, $N = 300$, and the electron initially very close to the eigenstate $E_e = -1$. In Fig. 10(b), we show the time evolution of the lattice energy. It exhibits periodically placed spikes and it becomes zero between them with a maximum value $E_{\ell,\max} = 0.0041$. The interaction energy [Fig. 10(c)] follows the same pattern with a maximum value $E_{e\text{-}\ell,\max} = 0.0026$. In Fig. 10(d), we show the time evolution of the electronic energy. The maximum transfer of energy from the electron to the lattice and interaction energy is 0.0067 at the spikes but all this energy is recovered between them. The participation number P is shown in Fig. 10(e) as it evolves in time. Even though it is a very sensitive function of any fluctuation in the wave function, it returns to its initial value [$P(0) = 300$] with impressive regularity and accuracy. The recurrence time (period) T_r, for this specific example shown in Fig. 10,

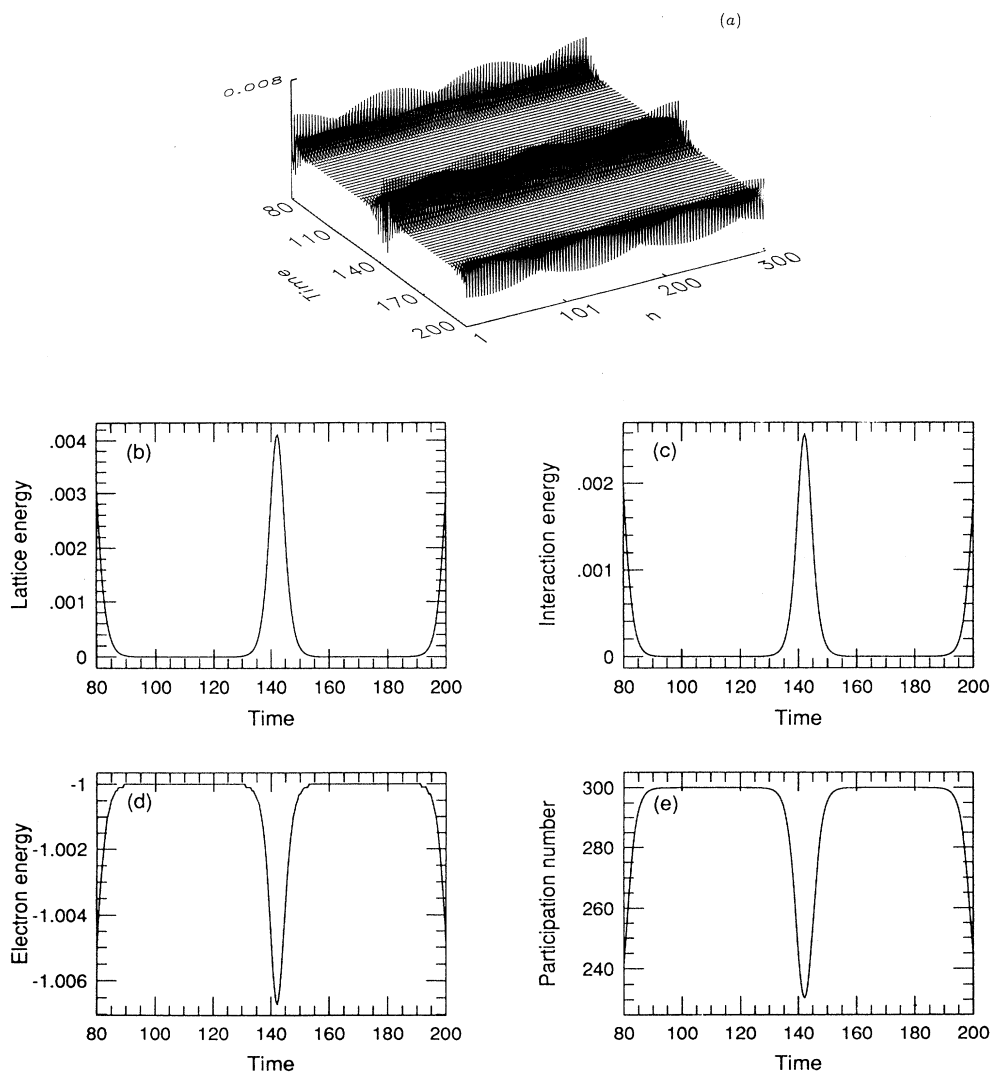

FIG. 10. The recurrence phenomenon for a system with $N = 300$, $t_e/t_\ell = 0.012\,24$, $\chi = 1.5$ in a relatively small time interval that illustrates the modulation and demodulation of the wave function together with the corresponding recurrence: the time evolution of the electronic wave function $|c_n(t)|^2$ (a), the lattice energy (b), the interaction energy (c), the electronic energy (d), and the participation number (e) are shown. The unit of time is t_ℓ and of energy is J. This behavior repeats itself for hundreds of recurrence periods without any sign of deterioration.

is $T_r = 60t_\ell$. This recurrence phenomenon is robust for small changes in the parameters and in the initial conditions. It is observed for electronic eigenstates close to $E_e \simeq -1$, for N in the vicinity of 300, and it survives in the region $1.35 < \chi < 1.58$ and $0.007 < t_e/t_\ell < 0.019$. It also seems to be persistent and stable (we run simulations for about $10^4 t_\ell$ and small perturbations do not destroy it). There is a strong dependence of the recurrence time (T_r) on χ, ranging from $T_r \sim 600t_\ell$ to $45t_\ell$ as χ increases within the above range. In Figs. 11 and 12, we show how the recurrence time (T_r) and the maximum lattice energy ($E_{\ell,\max}$) depend on the coupling (χ) and the electron mass (t_e/t_ℓ), respectively, for the region of the parameter space in which recurrence appeared. The strong dependence of T_r on the coupling constant (Fig. 11) shows that the phenomenon is due to the nonlinearity of our model and excludes linear resonance type of explanations. As we approach the lower quasicritical value of χ ($\chi \simeq 1.35$) the recurrence period becomes extremely long and the maximum value of E_ℓ and $E_{e\text{-}\ell}$ extremely low. The recurrence seems to disappear and the system apparently remains in its initial state. As we approach the upper quasicritical value ($\chi \simeq 1.57$) the phenomenon deteriorates after a few regular recurrence periods and eventually an apparently chaotic behavior is reached with considerably larger values of $|E_\ell|$, $|E_{e\text{-}\ell}|$, and $|E_e(0) - E_e|$. As far as the dependence of the phenomenon on the ratio t_e/t_ℓ is concerned, there are two distinct regimes (Fig. 12). For $t_e/t_\ell \geq 0.0115$, the behavior is as in Fig. 11—i.e., T_r decreases as t_e/t_ℓ increases—while $E_{\ell,\max}$ increases with t_e/t_ℓ. The recurrence disappears for $t_e/t_\ell \simeq 0.019$ in a very similar way as for $\chi \simeq 1.57$ described before. However, for $t_e/t_\ell \leq 0.0115$, the dependence of T_r and $E_{\ell,\max}$ are opposite: T_r increases and $E_{\ell,\max}$ decreases with increasing t_e/t_ℓ. Also, in this region, as opposed to the region $t_e/t_\ell \geq 0.0115$, the interaction energy ($E_{e\text{-}\ell}$) is negative and about equal in magnitude with the lattice energy, so that the electron energy changes very little.

The time evolution of the electronic wave function [Fig. 10(a)] and of the atomic displacements and velocities clearly indicates that the periodic transfer of energy back and forth from the electronic modes to the vibrational

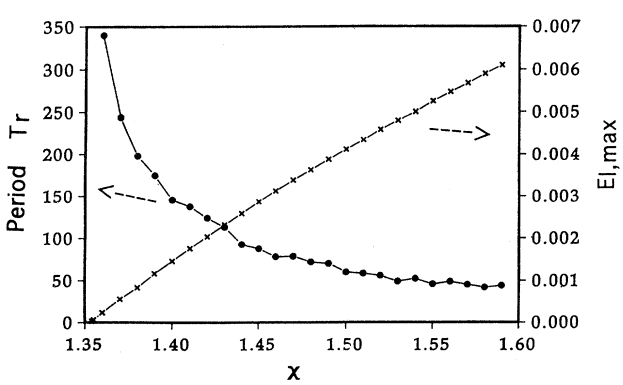

FIG. 11. The recurrence period T_r (solid circles) and the maximum lattice energy amplitude $E_{\ell,\max}$ (×) as a function of the electron-phonon coupling χ for a system with $N = 300$ and $t_e/t_\ell = 0.01224$.

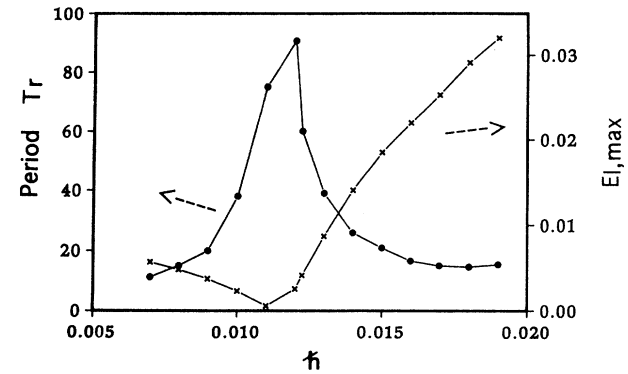

FIG. 12. The recurrence period T_r (solid circles) and the maximum lattice energy amplitude $E_{\ell,\max}$ (×) as a function of the ratio $t_e/t_\ell = \hbar$ for a system with $N = 300$ and $\chi = 1.5$.

modes corresponds to periodic modulation and demodulation of the wave function. In other words, the electronic wave function is not a simple Bloch state any more, but in addition to the "carrier" wave number corresponding to this eigenstate, a wave envelope develops. When it reaches maximum modulation, $|E_e - E_e(0)|$, $|E_{e\text{-}\ell}|$, and $|E_\ell|$ reach their maximum value, and when it demodulates, the energies return to their initial value [Figs. 10(b)–10(d)]. Similarly, P reaches a minimum value ($P = 230$) and returns to the initial value ($P = 300$) of the uniformly extended state [Fig. 10(e)]. This time evolution of the electronic wave function and the lattice degrees of freedom can be described approximately by solutions that consist of products of Jacobian elliptic functions and trigonometric functions. These approximate solutions (for the real part of the electronic wave function and the lattice displacements, for example) are

$$Re\ c_n = \frac{1}{\sqrt{N}} \cos\left(\frac{\pi}{3}n - \omega t\right) + C_1 \mathrm{cn}(\lambda t|\kappa) \cos\left(\frac{2\pi}{N}n + \frac{\pi}{3}n + \omega' t + \omega t\right), \tag{23}$$

$$u_n = C_2 \mathrm{cn}(\lambda t|\kappa) \cos\left(\frac{2\pi}{N}n + \frac{2\pi}{3}n + \omega' t + \varphi\right), \tag{24}$$

where $\hbar\omega = E_e(0) = -1$, $\pi/3$ is the initial Bloch wave number [corresponding to $E_e(0) = -1$], C_1 and C_2 are the modulation amplitudes, λ is related to T_r, κ (the modulus) is almost unity, $\omega' = 2\pi/T'$, $T' \simeq 2.64t_\ell$, and φ is a parameter-dependent phase. The intermediate frequency ω' seems to be independent of the parameters χ and t_e/t_ℓ. In Fig. 13, we compare the numerical values of $\mathrm{Re}c_n$ at a fixed time [Fig. 13(a)] with those of Eq. (23) [Fig. 13(b)]. Although the fit is satisfactory and the above expressions reproduce correctly the energies and participation number time dependence, they are not exact solutions of the equations of motion (7) and (8) for any value of the parameters and the initial conditions. It is interesting that these expressions have a similar form as a class of exact solutions of the integrable continuous

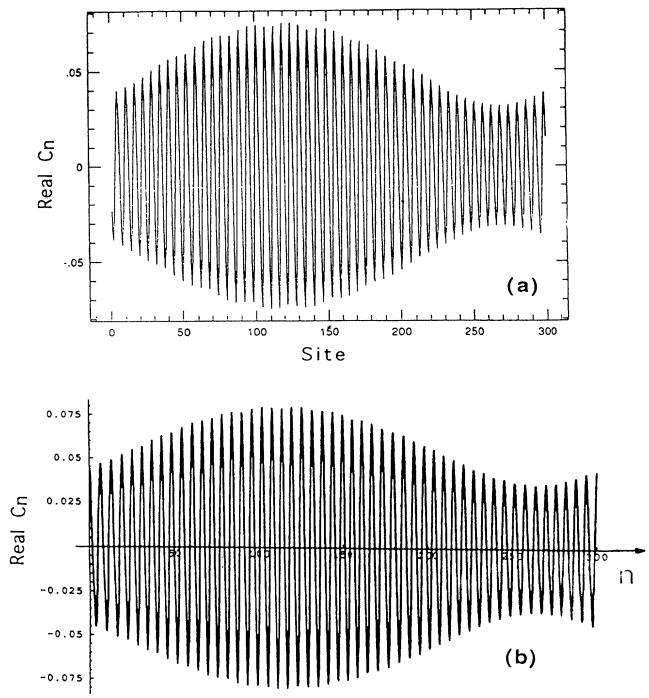

FIG. 13. The real part of $c(n)$ for a time moment from the numerical simulation in (a) and from the approximate solution [Eq. (23) in the text] in (b).

NLS equation[10] and some integrable version of the DNLS equation.[26]

The appearance of these solutions is related to the instability of the initial Bloch eigenstate which is necessary in order to drive the system away from this metastable state. When the parameters are in the appropriate range, any small perturbation to the eigenstate drives the system out of the initial state, leading eventually to the recurrent behavior. It should be pointed out that a similar recurrence resulting from a Benjamin-Feir instability[29] has been found both numerically and experimentally for the NLS equation,[30–32] but the initial state giving rise to the recurrence of our model does not necessarily satisfy the conditions obtained from linear and nonlinear stability analyses for the NLS equation.[8,9,33] Moreover, our model fully includes a large number ($N = 300$) of vibrational degrees of freedom in addition to the electronic degree of freedom, making the existence of such a regularity more unexpected in terms of a normal thermodynamic behavior. All of the above clearly suggest a torus of almost integrability interpretation of our results. It is possible that for this small region (and perhaps for other small regions as well) of parameter space our system exhibits local integrability or it is very close to being integrable.

V. CONCLUSIONS

We considered the discrete deformation potential model, which is one of the standard models that describe the interaction of the electrons with the lattice vibrations. We restricted ourselves to the case of a single electron in an otherwise empty band. We studied the time evolution of the coupled system numerically for several initial conditions, different coupling strengths, and electronic masses. In some cases the behavior predicted by approximate analytical methods has been recovered but, in the most part, a much richer and complex picture has emerged. Some states, with most impressive being the recurrent one, have been found. These solutions need further investigation in order to determine whether they reflect real physical properties of electron-phonon systems or are simply some newly discovered features of this particular, but widely used, model. The only approximation employed is the classical treatment of the lattice (at no point do we resort to the adiabatic approximation) which is certainly justified in the adiabatic regime but is more difficult to justify in other cases. However, our results recapture the main characteristics of electron-phonon systems in all cases. Naturally it would be desirable to treat both the electron and the lattice quantum mechanically and at the same time obtain an accurate time evolution of a highly excited state of the system, but this task is well beyond the current state of the art. Our approach allows systematic corrections when some of the quantum mechanical aspects of the lattice motion are taken into account.

In the work presented here we focused on the effects of varying the electronic effective mass (adiabatic parameter). We basically used two different types of initial conditions, the electron localized in k space (in an eigenstate) and the electron localized in real space (at a single site).

When the electron is initially close to an eigenstate, then, at the bottom of the band, increasing the effective mass does not favor localized polaron formation. On the contrary, for initially highly excited states, polaron formation becomes easier when the electronic mass becomes of the order of the atomic mass. But, in general, an increase of the initial electronic energy decreases the ability of the system to reach a localized state. A simple argument based on matching the electronic and atomic velocities explains these gross features of our results.

In the case of electrons initially localized at a single site the final state is extended, if the effective mass is small, and remains localized, if the effective mass is large and the coupling sufficiently strong. This behavior can be understood with the small polaron formation criterion.

The results of our extensive simulations of the dynamical behavior of the system determine the role of the parameters involved in this nonlinear coupled electron-lattice model and show how strongly the final state depends on the electronic effective mass and on the initial electronic configuration. This dependence is very interesting in the disordered case as well (results will be presented in a future publication). It is possible that this behavior will be significantly modified when temperature effects are included (this work is under way).

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