Polarons in a one-dimensional quasiperiodic model

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We considered the coupled motion of an electron described by a one-dimensional (1D) tight-binding Hamiltonian, whose diagonal matrix elements have a spatial variation incommensurate with the lattice, and a harmonic 1D lattice. The coupling was taken to be of the deformation-potential type. We studied numerically the time evolution of the coupled system starting with the lattice in its classical ground state and the electron in various initial states. Depending on the initial energy of the electron, on how close to the mobility edge it is and the strength of electron-lattice coupling, we found different types of localized and apparently extended (large) polarons. Near the mobility edge even a very weak coupling suffices to create a localized polaron even for high initial electronic energies. In many instances and even for very long times the electron does not seem to transfer much of its energy to the lattice.

I. INTRODUCTION

The question of polaron formation has been studied extensively over the last decades (for a recent review of the formal aspects of the problem, see Ref. 1). The emphasis has been on three-dimensional (3D) ordered systems. For these systems Emin and Holstein,[2] by omitting the kinetic energy of the lattice, have shown through a simple and elegant argument that the ground state of the coupled electron-lattice system is either an extended Bloch-type function (when the coupling strength is below a critical value) or (if the critical value of the coupling is exceeded) a collapsed atomic size state where the electron has been trapped permanently by a strong local lattice deformation. This basic result follows from the observation that the kinetic energy of the electron is proportional to $1/R^2$, while its interaction energy with the lattice goes as $-1/R^d$ (assuming a short-range electron-lattice interaction), where $R \geq a$ characterizes the linear extent of the electronic ground state, a is the lattice spacing, and d is the dimensionality. Thus, for $d=3$, the minimum total energy is obtained either for $R=\infty$ or for $R \approx a$, depending on whether $E(a) \gtrless 0$, where $E(R)$ is the total electronic energy. Hence, Emin and Holstein's basic results follow immediately. From the above argument, it follows also that for $d<2$, there is always a finite value of R, $R=R_0$, at which $E(R_0)$ has an absolute minimum. R_0 varies continuously from infinity towards the atomic size as the strength of the coupling increases from zero. It must be noted also that the above simple arguments break down if the interaction is long range as in polar crystals. In such cases intermediate size polarons appear for three dimensions as well.[3,4] If the lattice kinetic energy is turned on, one expects that the $R_0=\infty$ (or the very large R_0) electronic states would excite lattice vibrations and as a result would surround themselves by a cloud of phonons. The net result according to this picture would be a lowering of electronic energy by $\alpha\hbar\omega_L$ (where α is a measure of the electron-lattice coupling and $\hbar\omega_L$ is the characteristic energy of the longitudinal phonons surrounding the electron) and an increase of the electronic effective mass by a factor of $1+\alpha/6$.

This almost Bloch-type electronic state, together with the associated cloud of phonons, is referred to as a large polaron. The turning on of the lattice kinetic energy in a perfect periodic system, allows in principle the small polaron to move from site to site and to form a very narrow band. In practice, even a small amount of disorder is sufficient to keep the small polaron immobile and only at rather high temperatures thermally activated hopping allows the small polaron to move. The polaron formation picture outlined above, besides the various approximations involved in the relevant quantitative calculations, leaves out some very important aspects of the problem, as follows.

(i) The explicit role of the *disorder*: Of particular interest is the behavior near the so-called mobility edge, where the electronic states (in the absence of *el-ph* interaction) change from extended to localized. This problem has been addressed by Cohen *et al.*,[5] they found, by making use of the fractal character of the eigenfunctions near a mobility edge and by following an approach similar to that of Emin and Holstein,[2] that intermediate size localized polarons are formed in the vicinity of the mobility edge even for very weak short-range *el-ph* interaction. This result, if it is proved correct, has significant consequences because it effectively shifts the mobility edge into the region of extended states and thus changes the character of the metal-insulator transition from a power law to a discontinuity for the conductivity; the net result[5] is to restore the concept of a minimum metallic conductivity championed by Mott and Davis[6,7] and supported by experimental evidence. It should be mentioned that Phillpot *et al.*[8] have studied the effects of isolated impurities in the framework of the Su-Schrieffer-Heeger (SSH) Hamiltonian,[9] Anderson[10] also considered the case of electron-intramolecular phonon coupling in the presence of a site impurity.

(ii) The transient behavior: Of particular interest is the time evolution of a single electron initially photoexcited

or injected in an otherwise empty band as it interacts with the lattice. The response of an already formed polaron to the sudden or gradual application of an external electric field is also of great interest. Even if the *el-ph* interaction is so strong as to collapse a whole electronic band into a very narrow small polaron band, the latter obviously does not exhaust the Hilbert space available to the combined electron-lattice system. The initial unperturbed band is an excited subspace of the system. One main question is through what processes, if at all, initial spaces belonging to this excited subspace end up in the small polaron subspace. The possibility that the system may reach, under certain conditions, novel long-lived metastable states is an intriguing one, which may have remarkable physical consequences.

In the present work, we attempt to give some answers to these questions by examining a very simple system of an electron moving in and interacting with a 1D harmonic classical lattice. The 1D feature was chosen, in spite of its obvious shortcomings, because it greatly simplifies the numerical work. The electronic part of the Hamiltonian is a tight-binding model with the diagonal matrix element ε_n given by $\varepsilon_n=\varepsilon_0\cos(2\pi\sigma n)$, where σ is an irrational number. This choice of ε_n allows both extended and localized electronic eigenstates (depending on whether or not ε_0 is below a critical value). From this point of view our 1D model mimics the behavior of electrons in 3D disordered systems. The classical treatment of the lattice is an approximation, the consequences of which on the polaronic behavior are difficult to estimate. The coupling is typical for nonpolar materials.

The time evolution of our coupled model is described by a nonlinear system of differential (in time)—difference (in space) equations. As the ionic mass tends to zero, or for steady states, this system is reduced to the so-called discrete nonlinear Schrödinger equation.[11,12] The latter is known to sustain soliton solutions that are the analogs of intermediate or small polarons in our model. Given the complex behavior of the discrete nonlinear Schrödinger equation and the additional essential complication due the introduction of a new time scale characterizing the ionic vibrations, one expects that our model would exhibit a very rich behavior, which makes almost mandatory the use of numerical solutions. In all of our simulations we have taken the lattice as having initially zero kinetic and potential energy consistent with our picture of the electron having been injected or photoexcited in an otherwise empty and undisturbed band at very low temperatures. By following the time evolution of such initial states of the coupled system, we found, besides conventional large and small polarons, other more complicated steady states as well as situations where a steady state has not been reached. This rich variety of behaviors depends not only on the strength of the electron-phonon coupling, but very strongly on the initial electronic energy and on how close to the mobility edge the system is.

It must be pointed out that our approach can easily be extended to handle the problem of two electrons interacting with each other and with the lattice. Thus it allows a more accurate and detailed treatment of the question of bipolaron formation, especially in the poorly understood case where electron and ion masses are of similar magnitude or in the presence of anharmonic vibrations. This case may be relevant to narrow-band high T_c superconductors (see, e.g., Micnas, Ranninger, and Robaszkiewicz[13]) or to the newly discovered fullerides.[14]

In Sec. II we present our model and comment on its advantages and shortcomings. In the next section we introduce and discuss several quantities that seem useful in characterizing the morphology of the various types of polarons. We present also a brief outline of our method of numerical calculations. In Sec. IV we present and discuss our results and in the final Sec. V we summarize our main conclusions.

II. MODEL

The Hamiltonian describing our model is

$$H=H_e+H_l+H_{e-l} \ . \tag{2.1}$$

The electronic part H_e is taken to be a tight-binding model with diagonal matrix elements ε_n and nearest-neighbor matrix elements $-V\,(V>0)$, i.e.,

$$H_e=\sum_n \varepsilon_n |n\rangle\langle n| - V\sum_{nm}{}' |n\rangle\langle m| \ , \tag{2.2}$$

where the sites $\{n\}$ $(n=1,\ldots,N)$ form a 1D lattice with lattice constant a and periodic boundary conditions $|N+1\rangle=|1\rangle$; $|n\rangle$ is the local atomiclike orbital centered at the site n $(n=1,\ldots,N)$; the prime in the summation in (2.2) indicates that n and m are nearest neighbors. The quantities ε_n are given by

$$\varepsilon_n=\varepsilon_0\cos(2\pi\sigma n) \ , \tag{2.3}$$

where σ is an irrational number taken as the golden mean: $\sigma=(\sqrt{5}+1)/2$. Since σ is not a rational number, the Hamiltonian H_e is not periodic. This Hamiltonian, defining what is usually called a quasiperiodic model, has been studied extensively.[15–18] Its main characteristics are: (i) The spectrum develops infinitely many gaps, which become wider and wider as ε_0 increases (see Fig. 1), creating thus a pointlike structure; (ii) all the eigenfunctions are extended (i.e., nondecaying) for $\varepsilon_0/V<2$ and localized for $\varepsilon_0/V>2$; (iii) as the critical point (the so-

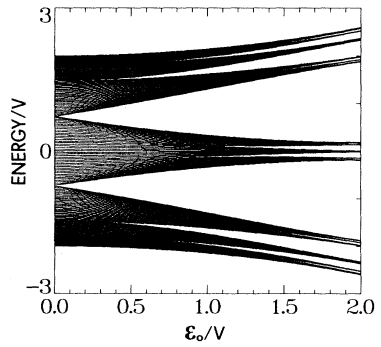


FIG. 1. Energy-level diagram for the quasiperiodic one-dimensional Hamiltonian as a function of the strength of the incommensurate term. The number of sites N is taken as 377.

called mobility edge) $\varepsilon_0/V=2$ is approached from below, the eigenfunctions develop strong fluctuations characterized by a length ξ, beyond which the eigenfunctions look uniform; (iv) in the localized regime ($\varepsilon_0>2V$), one defines an average decay length l_d; both ξ and l_d blow up at the critical point as $1/|(\varepsilon_0/2V)-1|$; (v) for length scales L, such that $a \ll L < \xi, l_d$ the eigenfunctions are fractal (more correctly, multifractal) objects[19,20] characterized by at least one fractal dimension D. The existence of mobility edges as well as the properties (iii)–(v) appear also in three-dimensional disordered systems. From this point of view our 1D quasiperiodic model simulates a real 3D disordered model. However, one should keep in mind that the "emptiness" in the spectrum of the present case does not appear in 3D disordered systems.

The lattice part of the Hamiltonian H_l is a simple classical harmonic one with acousticlike eigenvibrations

$$H_l=\frac{1}{2m}\sum_n p_n^2+\tfrac{1}{2}\kappa\sum_n (u_{n+1}-u_n)^2 , \tag{2.4}$$

where $p_n=m\dot{u}_n$ and u_n are the momentum and the displacement, respectively, of ion n, m is the ionic mass, and κ is the "spring" constant between nearest-neighbor ions. The maximum eigenfrequency of this Hamiltonian is $2\omega_0$ and the sound velocity is $c=\omega_0 a$, where $\omega_0=\sqrt{\kappa/m}$.

The electron-lattice interaction H_{e-l} is taken as a symmetrized deformation potential, i.e.,

$$H_{e-l}=\chi\sum_n |n\rangle\langle n|(u_{n+1}-u_{n-1}) . \tag{2.5}$$

The quantity χ is the strength of the coupling ($2a\chi$ is the so-called deformation potential). The Hamiltonian (2.5) couples the diagonal part of H_e with the lattice vibrations, in contrast with the SSH Hamiltonian,[9] which couples the off-diagonal part of H_e.

If the electronic wave function is written as

$$\psi_e=\sum_n c_n(t)|n\rangle , \tag{2.6}$$

with $\sum_n |c_n(t)^2|=1$, the equations of motion for the coupled electronic-lattice system become

$$i\hbar\dot{c}_n=[\varepsilon_n+\chi(u_{n+1}-u_{n-1})]c_n-V(c_{n+1}+c_{n-1}) , \tag{2.7}$$

$$m\ddot{u}_n=\kappa(u_{n+1}+u_{n-1}-2u_n)+\chi(|c_{n+1}|^2-|c_{n-1}|^2) , \tag{2.8}$$

while the electronic energy $E_e(t)=\langle\psi_e|H_e|\psi_e\rangle$ and the interaction energy $E_{e-l}(t)=\langle\psi_e|H_{e-l}|\psi_e\rangle$ are given by

$$E_e=\sum_n c_n^* c_n\varepsilon_n-V\sum_{nm}{}' c_n^* c_m , \tag{2.9}$$

$$E_{e-l}=\chi\sum_n c_n^* c_n(u_{n+1}-u_{n-1}) , \tag{2.10}$$

the lattice energy E_l is simply the Hamiltonian H_l.

The parameters of our problem are $\hbar$, V, and ε_0 for the electronic part, m and κ for the lattice part, and χ for the interaction part. If we choose V, m, and $\sqrt{m/\kappa}$ as the natural units of energy, mass, and time, respectively, then we are left with the following three parameters: (i) $\hbar$ (measured in units of $V\sqrt{m/\kappa}$, or equivalently the dimensionless quantity $\hbar/V\sqrt{m/\kappa}=(\hbar/V)/\sqrt{m/\kappa}=t_e/t_l$, where $t_e=\hbar/V$ and t_l are the characteristic electronic and lattice times, respectively); (ii) χ (measured in units of $\sqrt{V\kappa}$, or equivalently the dimensionless quantity $\chi/\sqrt{V\kappa}$, which is the square root of the quantity $\lambda=\chi^2/\kappa V$, appearing in the theory of superconductivity); and (iii) ε_0 (measured in units of V, or equivalently, the dimensionless quantity ε_0/V). In our natural system of units, the unit of length is $\sqrt{V/\kappa}$. In the results reported here we have kept t_e/t_l constant $\approx 1/81.8$ and we varied $\chi/\sqrt{V\kappa}$ over a range from about 0.2 to about 3. (Typical values of $\chi/\sqrt{V\kappa}$ for metals vary from about 0.3 to about 1.3). The third parameter ε_0/V was varied from zero up to its critical value 2. (Typical values for our natural units are $V=1$ eV, $m=Am_u$, where A is the mass number and m_u the atomic mass unit, and $\kappa=50$ N/m). The value of t_e/t_l chosen here is typical for most metals; however, in vary narrow-band materials, this ratio may approach or even exceed unity. The behavior then could be considerably different; we shall report on this case in a separate publication.

In our studies we followed the time evolution of our coupled system starting with an initial state, such that the lattice is at rest and undeformed and the electron is in one of the following states.

(i) Single site (ss) state: $\psi_e(0)=|n_0\rangle$, with n_0 close to $N/2$ and such that $E_e(0)\approx 0$.

(ii) Five-site state: $c_n(0)=1/\sqrt{5}$, $-1/\sqrt{5}$, $1/\sqrt{5}$, $-1/\sqrt{5}$, $1/\sqrt{5}$ for five consecutive sites around the middle of the specimen and $E_e(0)\approx 0$.

(iii) Eigenstate of H_e with $E_e(0)\approx 0$.

(iv) Gaussian wave packet: $c_n=(1/\sqrt{2\pi\sigma})\exp[-(n-n_0)^2/2\sigma^2]$, with $\sigma=3$, $n_0\approx N/2$, and $E_e(0)=-1.949$.

(v) Uniform state: $c_n=1/\sqrt{N}$ for each n; the initial energy is very close to -2.

(vi) Various eigenstates of H_e with energy near the bottom of the electronic band.

The above variety of initial electronic states allowed us to examine the dependence of our results on the initial energy as well as on the shape of the initial electronic wave function.

It is interesting to study the same problem when the lattice is not initially at its ground state, but in internal thermal equilibrium corresponding to a finite temperature T. In this case one can examine, through our model, what is happening at elevated temperatures ($T\gtrsim\Theta_D$, where $\Theta_D=2\omega_0\hbar/k_B$ is the Debye temperature), at which our classical approximations for the lattice vibrations are fully justified. Furthermore, at low temperature ($T\ll\Theta_D$), one can mimic approximately the effects of the lattice zero-point motion by taking $T=T_{ZP}$ where

$$Nk_B T_{ZP}=\tfrac{1}{2}\sum_k \hbar\omega_k ,$$

which gives

$$T_{ZP}=\frac{1}{\pi}\Theta_D . \tag{2.11}$$

Results for a finite initial lattice temperature will be reported elsewhere.

III. QUANTITIES OF INTEREST AND METHODS OF CALCULATION

Our first interest is to find the morphology of the polaron as a function of time. At each instant t, this morphology is characterized by $\{|c_n(t)|^2\}$, $n=1,\ldots,N$ (which gives the shape of the electronic wave function) and by $\{d_n(t)\}$, $n=1,\ldots,N$, where $d_n=(u_{n+1}-u_{n-1})/2$ (which gives the deformation of the lattice). We would like to find out whether or not the polaron is localized, i.e., whether or not $|c_{n-\bar{n}}(t)|^2\to 0$ as $|n-\bar{n}|\to\infty$ sufficiently fast (e.g., exponentially) for all values of t larger than a certain number.

The quantity $\bar{n}\equiv\bar{n}(t)$ is defined as

$$\bar{n}(t)=\sum_n |c_n(t)|^2 n \ . \tag{3.1}$$

We would like also to see how the polaron is spreading out, if at all; for this purpose one may consider the quantity

$$x^2(t)=\sum_n |c_n(t)|^2(n-\bar{n})^2 \tag{3.2}$$

or the quantity

$$x_0^2(t)=\sum_n |c_n(t)|^2[n-\bar{n}(0)]^2 \ . \tag{3.3}$$

However, if the transient phenomena last much longer than t_l, as it happens in many instances, to extract useful information from x_0 or x about the steady state one must consider extremely long specimens (very large N), which makes the numerical procedures extremely laborious. Furthermore, because of large fluctuations with n and t in $|c_{n-\bar{n}}(t)|^2$, very large N is required in order to find out unambiguously whether or not the wave function decays.

A very convenient quantity to characterize the electronic wave function is the so-called participation number P, which is by definition

$$P(t)=\left\{\sum_n |c_n(t)|^4\right\}^{-1} \ . \tag{3.4}$$

Since the wave function is normalized, $P=1$ if the wave function is completely confined at a single site and $P=N$ if the wave function is uniformly extended over the whole length of the specimen. Thus $P(t)$ is a measure of how many sites participate at a given instance in the wave function. We found that when $P<N/5$ the state is quite probably localized.

One may also define a lattice participation number P_l as follows:

$$P_l(t)=\left\{\frac{1}{E_l^2(t)}\sum_n \varepsilon_{ln}^2(t)\right\}^{-1} , \tag{3.5}$$

where $\varepsilon_{ln}(t)$ is the symmetrized local lattice energy

$$\varepsilon_{ln}(t)=\tfrac{1}{2}m\dot{u}_n^2+\tfrac{1}{4}\kappa[(u_{n+1}-u_n)^2+(u_{n-1}-u_n)^2] \ . \tag{3.6}$$

For $t\geq t_l$, $P_l(t)$ is expected to follow $P(t)$ very closely.

The various energies $E_e(t)$, $E_l(t)=E_{lk}(t)+E_{ld}(t)$, and $E_{el}(t)$ are also very important in their own right as well as very useful in providing indirect information about the nature of the polaronic states. If the concept of the polaron as a well-defined quasiparticle is valid, one would be able to separate the total energy $E(t)=E_e(t)+E_l(t)+E_{e-l}(t)$ into a polaronic part, which would include E_e, E_{e-l}, and part of E_l, and the rest of E_l, E_l', which represents the energy transferred to the lattice in the process toward total thermodynamic equilibrium. E_l' is the energy that would remain in the specimen if the polaron (i.e., the electron together with the associated lattice vibrations) is driven out of the specimen by, e.g., an external electric field. When the initial electronic state is a ground state, E_l' is obviously equal to zero. But for higher initial electronics it is not clear how to isolate E_l' out of E_l.

In our numerical simulations N was chosen as a Fibonacci number ($N=377$ or $N=610$) in order to satisfy the boundary condition $\varepsilon_{n=0}=\varepsilon_{n=N}$ as accurately as possible. The time integration is based on the fourth-order Runge-Kutta method with a step equal to $2\times 10^{-6}t_0$, where $t_0\equiv t_l(t_l/t_e)$. The size of the step was such that during the numerical simulation, energy is conserved to an accuracy of 10^{-5} or better. The lattice subsystem satisfies periodic boundary conditions ($u_{N+1}=u_1$). The time t_0 was introduced, because it turned out that many interesting phenomena occur for t of the order of t_0 or larger.

IV. RESULTS AND DISCUSSION

Our numerical results suggest that polarons can be classified in three broad categories:

(1) Apparently extended or large polarons characterized by (i) an electronic wave function that extends over all sites of the specimen without a pronounced peak, (ii) a large participation number ($\gtrsim N/3$), and (iii) a very small value of $|E_{e-l}|$ in comparison with E_l (this implies that $-\delta E_e\approx E_l$, where δE_e is the change in the electronic energy). (2) Localized or self-trapped polarons characterized by (i) an electronic wave function that has one or more pronounced peaks and seems to decay away from them, (ii) a participation number that decreases with time (apart from short-time fluctuations) and reaches, at steady state, a small value ($\lesssim N/5$), and (iii) a relatively small or ever positive value of δE_e. (3) Intermediate resonancelike polarons: This third category is intermediate between extended and localized polarons and may disappear altogether in an infinite system and for an infinite time lapse. The main characteristics of the intermediate resonancelike polarons as they appear in our finite systems are (i) the electronic wave function has one or more peaks but it does not seem to decay as one moves away from the peak(s), (ii) the participation number, besides its short-term fluctuations, exhibits long scale oscillations and consequently it does not seem to reach a steady state; and (iii) the values of $-\delta E_e$, E_{e-l}, E_l are all of the same order of magnitude. For a finite system and for finite in-

tervals of observation the boundaries between intermediate resonancelike and localized polarons or between resonancelike and extended polarons are not well defined.

The time evolution of our coupled system exhibits very interesting features. (1) In most cases, strong short term fluctuations appear (at a scale comparable to t_l), which seem to be chaotic. There are also longer time variations (of the order of $t_0 \equiv t_l^2/t_e = 81.8t_l$ up to $10t_0$ or even longer). Thus, although our system in most cases seems to be at a chaotic regime, some long term regularities in most cases seems to be at a chaotic regime, some long term regularities may also appear. (2) The process of equalizing the electronic temperature to that of the lattice appears to be either nonoperational or very slow and dependent on the initial electronic wave function.

Our results are strongly dependent on ε_0 (i.e., on how close to a mobility edge we are) and on the initial electronic energy. Below we describe specific cases starting with those where the initial electronic energy is near the center of the band.

In Fig. 2 we show results for $\varepsilon_0 = 1$, $\lambda = 0.86$, $N = 3.77$, and a single site initial state with $E_c(0) \approx 0.015$. For an initial period ($t < 5t_l$) the lattice cannot respond to the electron and the latter propagates ballistically with $x^2 \sim t^2$ [Fig. 2(a)]. During this period the participation number grows roughly linearly (with some fluctuations) until it reaches a rather large value of about 190, indicative of an electronic state extended over the whole length of the specimen. After this initial period the electron-lattice interaction becomes operative but it is unable in the present case to self-trap the electron, which remains clearly extended, as can be seen in Figs. 2(b) and 2(c), where the unit of time t_0 is taken as $t_l^2/t_e \approx 81.8t_l$. It is interesting to notice the seemingly chaotic fluctuations of $P(t)$ around its average value of $P \approx 180$. These fluctuations do not decay with time. On the contrary, some larger and larger short term excursions towards smaller values of P appear as we follow the evolution of the system over long times. In Fig. 2(d) we show the E_l versus t. The first thing to notice is that only a small fraction of the available electronic energy (about 5%) has been transferred to the lattice in spite of the rather strong coupling ($\lambda \approx 0.86$) and the extremely long running time ($350t_0 \approx 3 \times 10^4 t_l$). One can use Fermi's golden rule to obtain the electronic collision time due to its interaction with the lattice (assuming that the electron and the lattice vibrations are quasiindependent degrees of freedom)

$$\frac{1}{\tau} = \frac{2\pi}{\hbar} \lambda \bar{U}_L \ , \tag{4.1}$$

where $\bar{U}_L$ is the time-average lattice energy per site

$$\bar{U}_L = \frac{1}{Nt} \int_0^t dt' E_l(t') \ . \tag{4.2}$$

For $t = 380t_0 = 3.1 \times 10^4 t_l$, our results show that $\bar{U}_L \approx 1.86 \times 10^{-4}$, $\tau = 12.2t_l$, and $t/\tau \approx 2550$. In spite of this very large ratio of t/τ, the quantity $A(t) = [E_e(t) - E_B]/[E_e(0) - E_B]$, where E_B is the lower band edge ($E_B \approx -2.18$ for $\varepsilon_0 = 1$), is only 0.845. Assuming that $A(t) = \exp(-t/\tau_{\text{in}})$, where $\tau_{\text{in}}(t)$ is the inelastic electronic relaxation time, we find that $t/\tau_{\text{in}} \approx 0.055$ or $\tau_{\text{in}}/\tau \approx 4.6 \times 10^4$. This extremely long effective inelastic relaxation time (which seems also to increase with time) is a very surprising result, since one would expect τ_{in}/τ to be at most of the order to $t_l/t_e \approx 81.8$. One possible explanation for this result is that part of the lattice energy is associated with the lattice vibrations dressing the bare

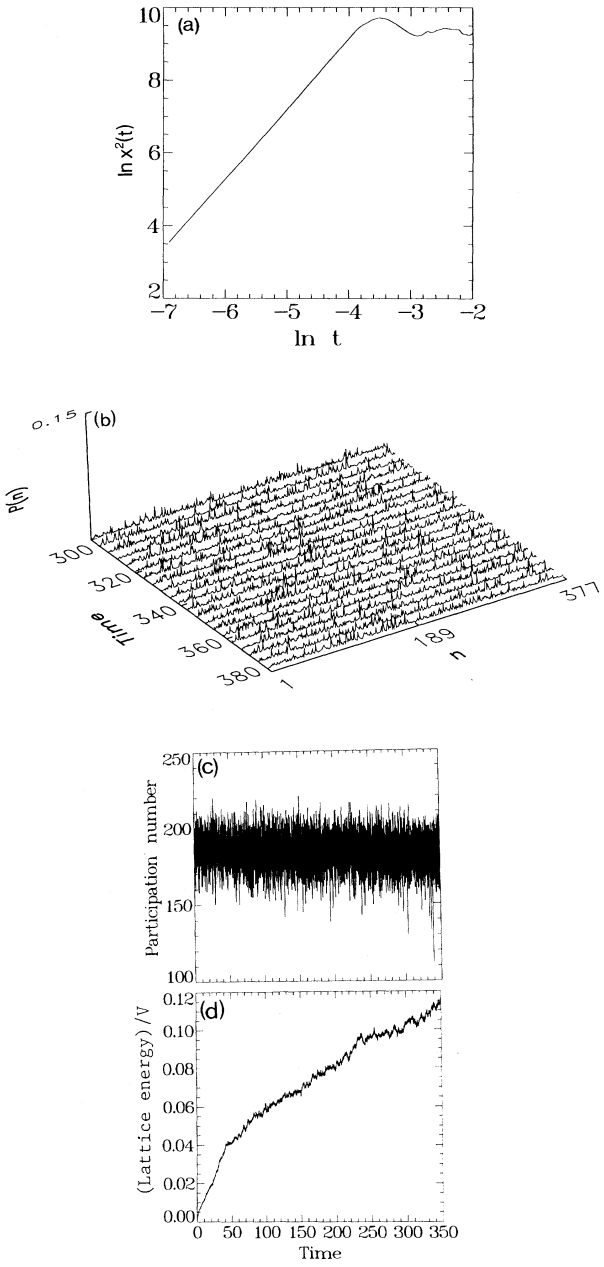


FIG. 2. Extended (large) polaron formation for a system with $\varepsilon_0 = 1$, $\lambda = 0.86$, $N = 377$. The initial electronic state is a single-site one with $E_e(0) = 0.015$. The unit of time is $t_0 = t_l^2/t_e = 81.8t_l$, length is the lattice spacing, and energy is V. Panel (a) shows $\ln x^2$ vs $\ln t$ (the saturation at $\sqrt{x^2} \approx 128$ is due to the finite size of the system). The time evolution of the electronic wave function is also shown (b), as well as the participation number (c), and the lattice energy (d). $P_n(t) \equiv |c_n(t)|^2$.

electron to form the polaron. Once the polaron is formed it may interact perhaps very weakly with the lattice through a renormalized coupling $\lambda_R \ll \lambda$. This assumed weak coupling, together with a reduction of the effective $\overline{U}_L$ (due to the fact that the polaron is not scattered by its own cloud of lattice vibrations) may possibly account for the surprising result of very slow and very weak transfer of energy from the electron to the lattice. Another mechanism for this slowdown of the relaxation of the electronic energy may be associated with the breakdown of the spectrum in subbands separated by rather large gaps (see Fig. 1). The electron, according to this explanation, relaxes until it reaches the bottom of the subband(s). Further relaxation would require nth order processes, where n is a large number of the order of $E_g/2\hbar\omega_0$ and E_g is the relevant gap. These higher-order processes are extremely slow if $\lambda E_l(t)/E_g$ is much smaller than unity. This explanation may account for the fact that ss initial electronic wave function transfer energy to the lattice at a much slower rate than the eigenstates of the same energy (middle of the band). Indeed, the ss state is a linear combination of all eigenstates of the system and consequently the slowdown must start when the bottom of the narrowest band is reached and proceed in a hierarchy of slower and slower relaxation times as the bottoms of wider bands are reached; on the contrary, the eigenstate with $E_e \approx 0$ is associated with the central band, which is the widest, and consequently, the slowdown there will be delayed. However, detailed examination shows that the time dependence of $E_l(t)$ and $E_e(t)$ does not quite fit the above expectations (e.g., a case of $\varepsilon_0=1$, $\lambda=9,6$) and the ss initial state seems to saturate at $E_l \approx 0.4$, for which $\lambda E_l/E_{g,\max} \approx 4.3$, and as a result one expects that the fragmentation of the spectrum does not really matter since higher-order processes would proceed as fast as the first-order ones. Furthermore, for the same values of ε_0 and λ but for an initial eigenstate with $E_0 \approx 0$, E_l equals 0,8 already at $t=10t_0$ and continues to increase, while the half bandwidth of the central band is only 0.35. Possibly a combination of the dressing mechanism (mentioned before) and the fragmentation of the spectrum is at work in the present model to prevent the expected relaxation of the system.

In any case, our results suggest that even for relatively long times [of the order of $(10^5-10^6)t_l$] an electron excited near the center of the band would transfer very little of its energy to the lattice at very low temperatures (a few degrees K), assuming, of course, that the quantization of the lattice vibrations would not change this conclusion qualitatively. Although equipartition of energy between the electronic and the lattice degrees of freedom did not occur in the present case, the lattice itself seems to be in internal thermodynamic equilibrium because the lattice kinetic and potential energies are equal (apart from short term chaotic fluctuations, which are quite appreciable of the order of 20%). Very strong and growing with time chaotic fluctuations appear also in $E_{e-l}(t)$, which on the average remains very small [$E_{e-l}(t) \approx -0.002$, i.e., about 2% of E_l, while $|\delta E_{e-l}|/E_{e-l} \approx 1$]. Thus the case of Fig. 2 presented above has all the characteristics of an extended or large polaron. It is worthwhile to note that the E_l versus t exhibits several characteristic times ($t_1 \approx 2t_0 \approx 160t_l$, $t_2 \approx 45t_0 \approx 3680t_l$, and possibly $t_3 \approx 250t_0 \approx 20000t_l$), at which the slope of curve changes to lower values. A possible interpretation of this result is that the dressing of the bare electron occurs at discrete steps and that the interaction of a partially dressed electron (i.e., a partially formed polaron) with the lattice is only partially reduced. An alternative interpretation of this hierarchy of relaxation times may be relaxed with the fragmentation of the unperturbed spectrum as mentioned before. Note, however, that this steplike polaron formation becomes quite obvious in cases of localized polarons, where the electronic energy E_e remains almost constant and consequently, does not reach a band edge.

In Fig. 3 we show a weak interaction resonancelike case near the boundary with the extended regime. The electronic wave function exhibits occasional pronounced peaks, which are mobile and not permanent. The participation number after its initial fast growth to a value of about 190 remains constant on the average, up to $t=t_1 \approx 20t_0 \approx 1600t_l$ a behavior typical of extended polaron. However, for $t > t_1$ a reduction in P appears accompanied by an increase of $|E_{e-l}(t)|$, and a change in the average slope of $E_l(t)$. This behavior is due to the formation of a pronounced (mobile) peak in the wave function. The gradual dissolution of this peak for $t > t_2 \approx 40t_0 = 3300t_l$ brings the values of P and E_{e-l} back to 180 and -0.015, respectively. However, both E_l and E_e appear to have reached saturation for $t \geq 30t_0 \approx 2500t_l$ ($E_l \approx 0.235$ and $\delta E_e = -0.22$, while $E_{e-l} \approx -0.015$). This apparently complete termination of energy transfer from the highly excited electron (effective temperature of the order of 20 000 K) to the low-temperature lattice degrees of freedom (effective temperature 7 K) is totally unexpected; one may be tempted to attribute this surprising result to a reverse flow of energy from the lattice to the electron during the dissolution of the pronounced peak. This reverse flow may temporarily compensate the natural flow of energy from the electron to the lattice. However, this possible explanation cannot be of general validity because we have studied another case [$\varepsilon_0=1.5$, $\lambda \approx 0.38$, $N=377$, ss initial wave function with $E_e(0) \approx 0.0245$] exhibiting all the typical characteristics of an extended polaron [$P(t) \approx 170$ for all $t \geq 10t_l$, $E_l \approx -\delta E_e$, $|\delta E_{e-l}|/E_l \approx 1\%$] without any pronounced peak(s), which nevertheless shows saturation of E_l and δE_e at 0.032 and -0.032, respectively, for $t \geq t_1 \approx 32t_0 \approx 2600t_l$. Notice also that the short term fluctuations are much more pronounced and chaotic for the electronic quantities (P, E_e, E_{e-l}) than for the total lattice energy (although the lattice kinetic and potential energy exhibit also strong chaotic fluctuations). We point out that the saturation value of E_l and E_e of the case shown in Fig. 3 are comparable to the half bandwidth of the spectrum, supporting thus the idea that transitions between subbands are practically forbidden.

In Fig. 4 we show a case that can be characterized as borderline between resonancelike and localized [$\varepsilon_0=1$, $\lambda \approx 9.5$ (extremely large), $N=377$, ss initial state with

$E_e(0)=0.015$]. The time evolution of the wave function is shown in Fig. 4(a); the two characteristic pronounced peaks, in spite of their changes in intensity, seem to be a permanent feature of the wave function. For middle of the band polarons, as opposed to band-edge polarons, the appearance of more than one peak in the wave function is a rather common feature. Figure 4(b) shows that the localized or resonancelike polaron is formed in steps (in the present case the steps occur at $t_1 \approx 10t_0 \approx 800t_l$ and $t_2 \approx 18t_0 \approx 1500t_l$); these steps show more clearly in the E_{e-l} versus t plot [Fig. 4(c)]. The rise in P and E_{e-l} for $t > 25t_0$ is due to the reduction of the strength of the peaks in the wave function. In the present case the lattice energy seems to saturate to a value of 0.4 ± 0.02, while $\delta E_e \approx -0.2\pm0.04$. We have also checked the dependence of the various features on the length of the specimen by repeating the calculation for $N=610$. We found that P/N is roughly independent of N as expected for an extended or resonancelike state. It takes a longer time for a steady state to be reached for $N=610$ (about three times longer) as compared with the $N=377$ case. At the steady state E_l, δE_e, and E_{e-l} seem to be independent of N. The time delay for the larger N case may be attributed to the ballistic ($x^2 \sim t^2$) spread of the initial

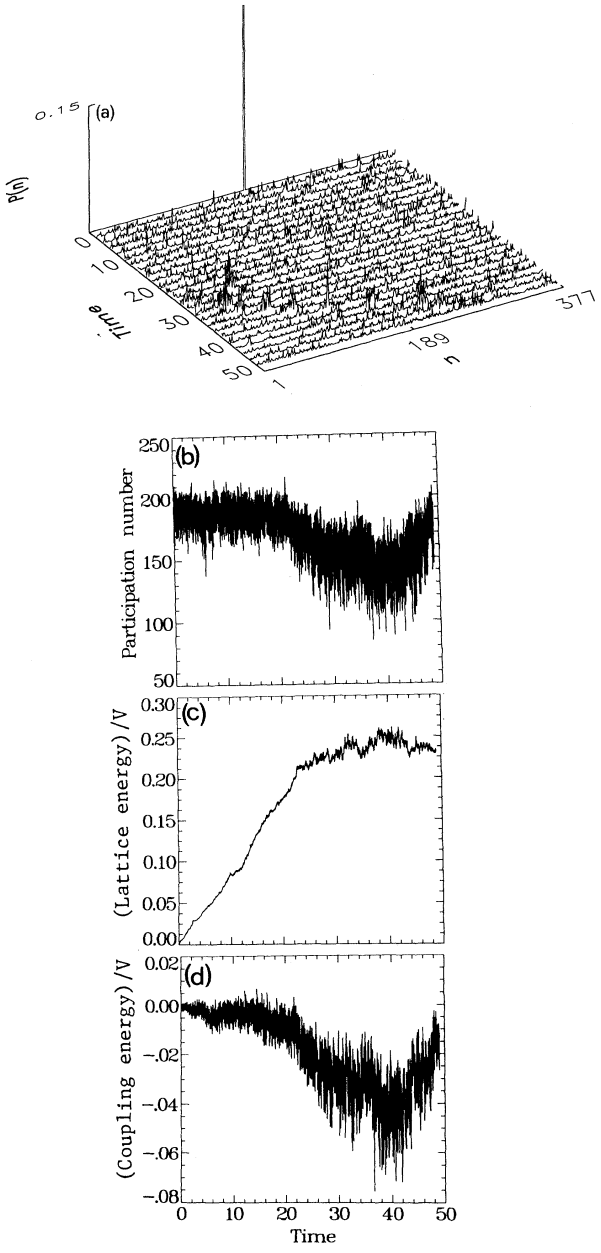


FIG. 3. Intermediate resonancelike polaron formation for a system with $\varepsilon_0=0.5$, $\lambda \approx 6$ (very strong coupling), $N=377$, and ss initial electronic state with $E_e(0)=0.008$. The unit of time is $t_0=t_l^2/t_e \approx 81.8t_l$ and energy is V. The time evolution of the electronic wave function is shown (a), together with the participation number $P(t)$ (b), the lattice energy $E_l(t)$ (c), and the interaction energy $E_{e-l}(t)$ (d). $P_n(t)=|c_n(t)|^2$.

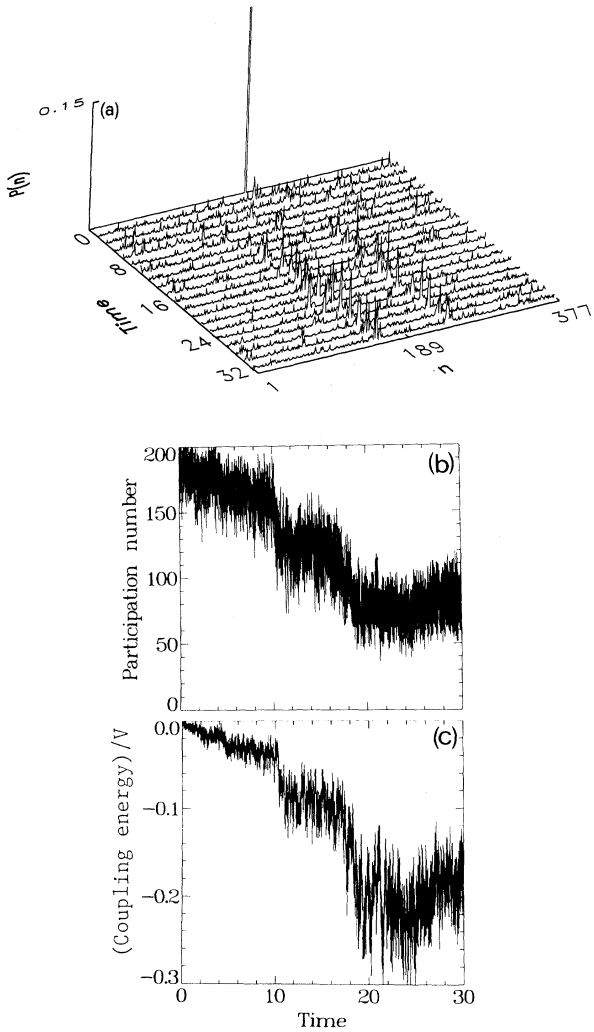


FIG. 4. Strong resonancelike polaron for a system with $\varepsilon_0=1$, $\lambda \approx 9.5$ (extremely strong coupling), $N=377$, and ss initial electronic state with $E_e(0)=0.015$. The unit of time is $t_0=t_l^2/t_e \approx 81.8t_l$. The time evolution of the electronic wave function (a), $P(t)$ vs t (b), and $E_{e-l}(t)$ (c), are shown. $P_n(t)=|c_n(t)|^2$.

electronic wave function over the entire length of the specimen before the electron-lattice interaction has the time to respond. Thus effectively when the interaction becomes operational the initial conditions are different for different N's, the quantity $\chi(|c_{n+1}|^2-|c_{n-1}|^2)$ (which acts as an external force on the lattice) is smaller for the longer system and consequently the longer system will require more time to reach a steady state. According to this argument, one expects that the N dependence may disappear or become much weaker if $N \gg 10t_l/t_e \approx 1000$, because in this case the electron-lattice interaction will become fully operational before the electron has a chance to reach the edges of the specimen.

A very interesting strong resonancelike or possibly localized state is shown in Fig. 5, where a clearly localized ($P \approx 30$) polaron is formed at $t_1 \approx 0.8t_0 \approx 65t_l$, which subsequently is dissolved with P jumping back to values around 140. Later on ($t_2 \approx 5.5t_0 \approx 450t_l$), a less pronounced peak is formed, causing P to drop below 100 and finally at $t_3 \approx 12.5t_0 \approx 1000t_l$ the peak becomes more pronounced with P saturating at 50 ± 15. This apparently localized polaron is not so robust as indicated by the rather strong fluctuations in P. It is worthwhile to note that in the present case the lattice energy initially ($5t_l < t < 130t_l$) increases linearly with t with an effective $\tau_{\text{in}} \approx 30t_0 \approx 2500t_l$, while in this period the average τ [calculated according to Eq. (4.1)] is about $30t_l$, the ratio τ_{in}/τ being about 83, i.e., quite close to the ratio t_l/t_e, as expected. At the end of the period ($t \approx 1.6t_0 \approx 130t_l$) the lattice energy is 0.11. However, for $2t_0 \approx 150t_l < t < 1500t_l \approx 20t_0$ the transfer of energy to the lattice slows down considerably (the effective τ_{in} *is now* 15 times larger than before), while at the same time τ *decreased* by a factor of 2. If the initial electronic state, instead of being an eigenstate with $E_e(0) \approx 0$, is a ss state [again with $E_e(0) \approx 0$], the transfer of energy to the lattice is much slower, e.g., for $5t_l < t < 250t_l \approx 4t_0$ the increase in $E_l(t)$ is almost linear with a $\tau_{\text{in}} \approx 300t_0 \approx 24\,000t_l$, i.e., an order of magnitude slower rate of transfer of energy. This strong dependence on the shape of the initial electronic state is surprising because in the ss case the electron very quickly spreads over the whole system (already at $t \approx 4t_l$, $P \approx 170$, i.e., about the same as the participation number of the eigenstate) and hence one would expect naively that from this point on both states would behave similarly. Another surprising feature worth mentioning is that at the initial period, $t < 4t_l$, where the lattice hardly affects the motion of the electron, the transfer of energy to the lattice takes place at the fastest rate ($\tau_{\text{in}} \approx 17t_0 \approx 1400t_l$ for the ss case). All these results indicate that the motion of the electron is highly correlated with that of the lattice and that memory of the initial conditions is retained in spite of the apparently chaotic fluctuations.

A clearly localized polaron [$\varepsilon_0 = 1.5$, $\lambda = 2.4$, $N = 377$, eigenstate with $E_e(0) \simeq 0$] is shown in Fig. 6 exhibiting a multiple peak structure [Fig. 6(a)] common in highly excited localized (or resonancelike) polarons. Figure 6(b) shows that the localized polaron is formed in two clearly defined steps at $t_1 \approx 2t_0 \approx 165t_l$ and $t_2 \approx 6t_0 = 500t_l$. For $t > t_2$ a steady state is reached with $P \approx 30 \pm 5$, $E_l = 0.37 \pm 0.03$, $\delta E_e = -0.12 \pm 0.02$, and $E_{e-l} = -0.24 \pm 0.04$. The second step at t_2 is associated with a rise in the electronic energy (which continues up to $1.5t_2$) due to a strong increase in the electronic kinetic energy as a result of the localization.

In Fig. 7 we show results for the critical point $\varepsilon_0 = 2$ [and $\lambda \approx 0.095$, $N = 377$, ss initial wave function with $E_e(0) \approx 0.034$]. In Fig. 7(a) the x^2 versus t is plotted; for short times ($t \leq 4t_l$), the behavior is diffusive ($x^2 \sim t$), as expected[21,22] for the critical point without electron-lattice coupling. For $t > 4t_l$, when the interaction becomes operative, the motion is subdiffusive ($x^2 \sim t^\beta$ with $\beta \approx 0.6$) up to $t \approx 1.2t_0 \approx 100t_l$, beyond which the curve bends over and finally saturates. The saturation value of

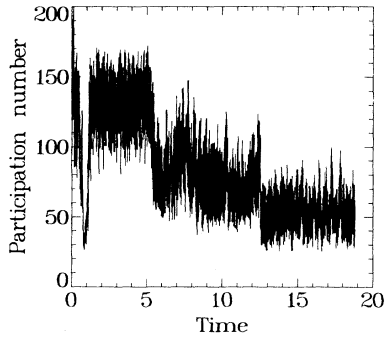
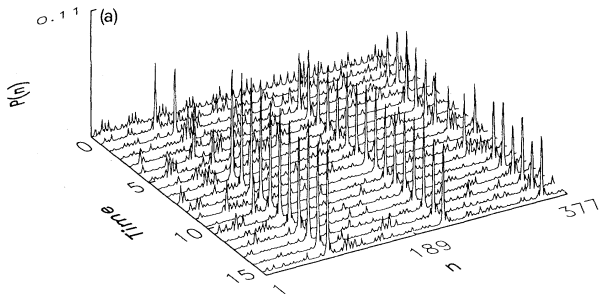


FIG. 5. $P(t)$ vs t for an intermediate resonancelike polaron with $\varepsilon_0 = 1.5$, $\lambda \approx 0.86$, $N = 377$, and initial electronic state, an eigenstate of H_e with $E_e(0) \approx 0$. The unit of time is $t_0 = t_l^2/t_e \approx 81.8t_l$.



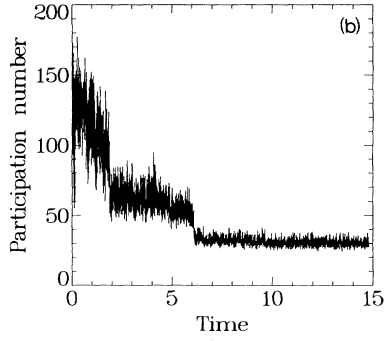


FIG. 6. Time evolution of the electronic wave function (a) and P vs t (b) for a localized polaron with $\varepsilon_0 = 1.5$, $\lambda \approx 2.4$, $N = 377$, and initial state, an eigenstate of H_e with $E_e(0) \approx 0$. The unit of time is $t_0 = t_l^2/t_e \approx 81.8t_l$. $P_n(t) \equiv |c_n(t)|^2$.

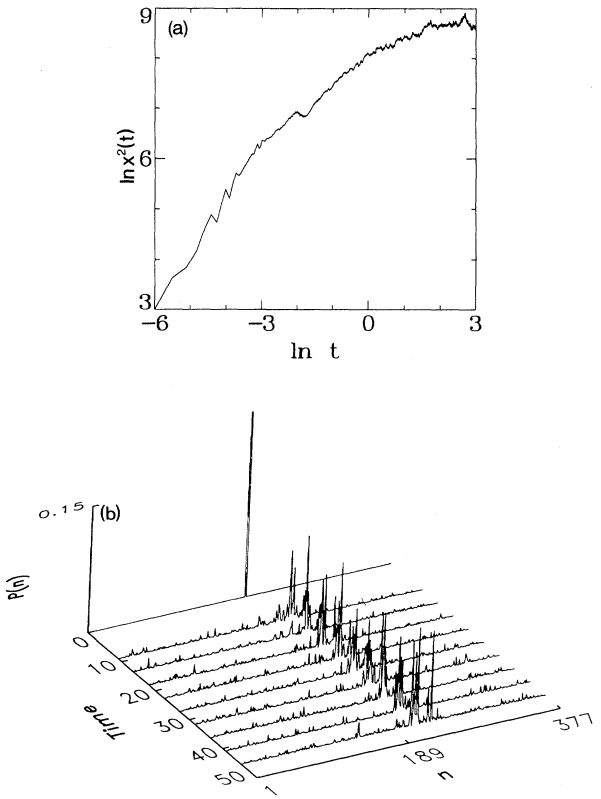


FIG. 7. x^2 vs t and time evolution of the electronic wave function for a localized polaron at the critical point $\varepsilon_0=2$ [$\lambda=0.095$, $N=377$ and ss initial state with $E_e(0)\approx 0.034$]. The unit of time is $t_0=t_l^2/t_e\approx 81.8t_l$. $P_n(t)=|c_n(t)|^2$.

$\sqrt{x^2}$ is about 75 comparable to the saturation value (80) obtained for $\lambda=0$. Thus we cannot say in the present case whether or not the saturation is due to the finite length of the specimen or the localization of the polaron. However, when we increased λ to 0.38 the saturation is due to the lattice-induced localization. In this last case there is also a subdiffusive regime with $\beta\approx 0.65$ between $t_1\approx 4t_l$ and $t_2\approx 2t_0\approx 150t_l$; beyond t_2 saturation sets in rather abruptly. In Fig. 7(b) we show the time evolution of the electronic wave function. An approximate steady state sets in after roughly $t\approx 2t_0\approx 165t_l$ with $P\approx 42\pm 10$, $E_l\approx 0.013\pm 0.002$, $\delta E_e\approx -0.007\pm 0.0005$, and $E_{e-l}\approx -0.005\pm 0.0015$.

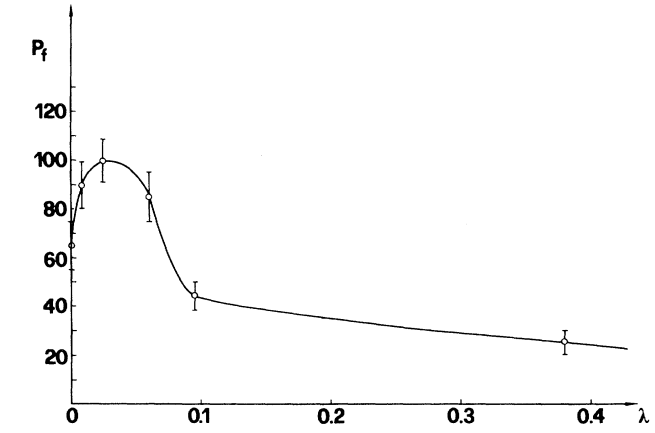


FIG. 8. Saturation value of the participation number P_f vs λ for a critical point ($\varepsilon_0=2$) polaron with $N=377$ and ss initial wave function with $E_e(0)\approx 0.034$. The solid line is a guide to the eye.

In Fig. 8 we plot the saturation value of P versus λ for the critical value of ε_0, $\varepsilon_0=2$, $N=377$, and ss initial wave function with $E_e(0)\approx 0.034$. P initially *increases* with increasing λ and then for $\lambda>0.05$ decreases monotonically with λ. We attribute this initial increase of P to a "phonon-assisted" smoothening of the very fragmented critical-point eigenfunctions. For larger λ the lattice-induced localization becomes stronger and squeezes the electronic wave function, thus giving rise to a smaller P.

In Fig. 9 we show a more conventional case of localized polaron in a periodic system ($\varepsilon_0=0$) starting from a lower band-edge eigenstate, namely, the uniform one with $c_n=1/\sqrt{N}$ (a very small departure from uniformity is necessary in order to drive the system out of the metastable state, $c_n=1/\sqrt{N}$, $u_n=0$ for all n and t). The electronic wave function has a smooth single peak with a half width that oscillates between about 20 and 30. The participation number oscillates between 30 and 43. The localized polaron formation is accompanied by an increase in the electronic energy (which being purely kinetic increases as a result of the confinement). This increase (which at maximum is $\delta E_e=0.004$) and the increase in the lattice energy ($E_l\approx 0.011$) are compensated by the electron-lattice energy, which reaches -0.015 at its minimum.

In Fig. 10 we show another case of weak-coupling localized polaron near the bottom of the band but for $\varepsilon_0=0.5$ (weak departure from periodicity). The wave function is not smooth anymore [Fig. 10(a)]. The P versus t plot [Fig. 10(b)] shows that the polaron is formed in a nonmonotonic way through the characteristic steps. A decaying oscillatory behavior, due to a breathing character of the localized polaron, is shown in Fig. 10(b) and more clearly in Fig. 10(c), where the sharp peak at $2.6t_0$, $7.5t_0$, $12t_0$, $16.6t_0$ (with a period of approximately 4.7) are associated with the maximum contractions of the polarons. These contractions appear as sharp dips in Fig.

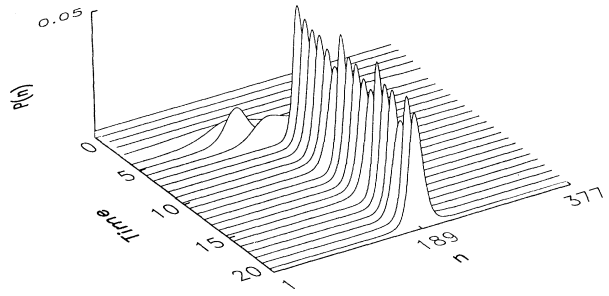


FIG. 9. Time evolution of the electronic wave function for a localized polaron in a periodic system ($\varepsilon_0=0$) with $\lambda=0.095$, $N=300$, and a uniform initial state with energy $E_e(0)=-2$ (i.e., at the bottom of the band). $P_n(t)\equiv|c_n(t)|^2$.

10(d). It is clear from Figs. 10(c) and 10(d) that other shorter periods are also present. Furthermore, the coupling energy $E_{e-l}(t)$ is considerably more noisy than the total lattice energy. It is worthwhile to mention that the electronic energy increases (δE_e reaches 0.004 at the maximum contraction and saturates at a value of 0.0018 ± 0.0008) again as a result of the increase of the kinetic energy due to the uncertainty principle.

In Fig. 11 we show the transition from a resonancelike polaron to a localized one as we increase the coupling constant λ. In panel (a) we show a typical case of a rather strong intermediate resonancelike polaron with the characteristic peaks that sometimes become very pronounced, then broaden and tend to disappear and reappear again at different positions. Associated with this erratic long term time evolution is the behavior of the participation number, which shows strong short and long term fluctuations: e.g., for $t_0 < t < 20t_0$, $P \approx 200\pm30$; for $21t_0 < t < 35t_0$, $P \approx 100\pm50$; for $37t_0 < t < 50t_0$, $P \approx 130 \pm 50$, etc. On the other hand, E_l, E_e, and to lesser degree E_{e-l}, seem to have saturated (apart from short term fluctuations) for $t > 21t_0$: $E_l \approx 0.043\pm0.003$, $\delta E_e \approx -0.038\pm0.002$, $E_{e-l} \approx -0.004\pm0.003$. In Fig. 11(b) we show a case of a marginally localized polaron. It takes a long time ($t \approx 15t_0$) for the characteristic peak to reappear; during this long period P is initially almost constant (for $2,5t_0 < t < 9t_0$, $P \approx 190\pm40$) then drops linearly with time. This linear reduction continues even after the formation of the peak up to $t = t_1 \approx 19t_0 \approx 1500t_l$.

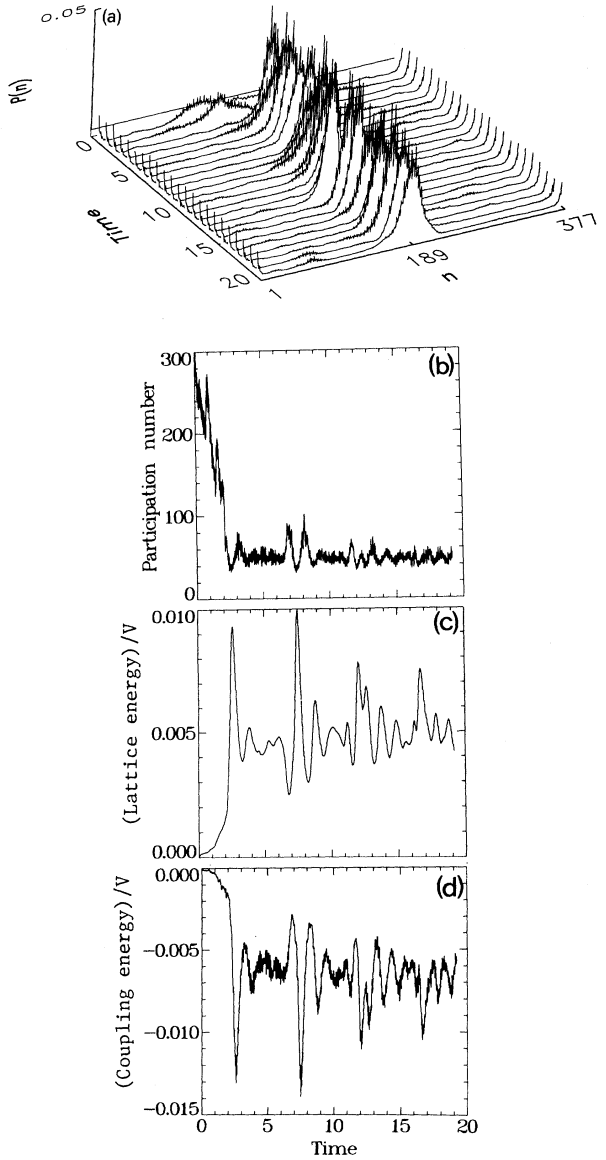


FIG. 10. Localized polaron formation near the lower band edge [$\varepsilon_0=0.5$, $\lambda=0.095$ (very weak coupling) $N=377$, uniform initial state with $E_e(0)=-2.001$]: (a) time evolution of the electronic wave function; (b) participation number; (c) lattice energy; and (d) interaction energy. The unit of time is $t_0=t_l^2/t_e\approx81.8t_l$. $P_n(t)=|c_n(t)|^2$.

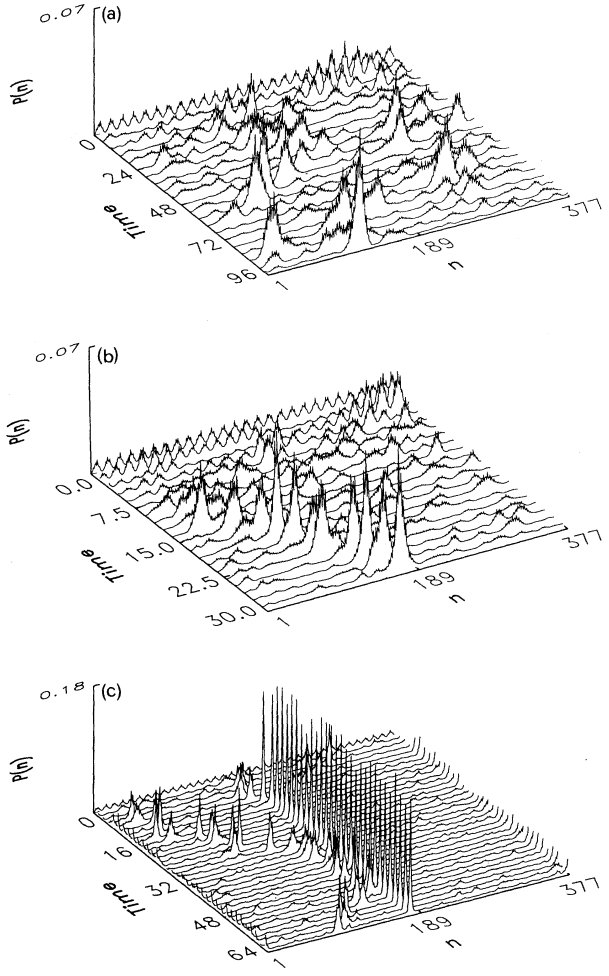


FIG. 11. Time evolution of the electronic wave function for $\varepsilon_0=0.5$, $N=377$, and (a) $\lambda=0.16$; (b) $\lambda=0.21$; and (c) $\lambda=1.52$. For cases (a) and (b) the initial wave function is the 27th eigenfunction of H_e (counting from the ground state up), while for case (c) the initial wave function is the 37th eigenfunction of H_e. The unit of time is $t_0=t_l^2/t_e\approx81.8t_l$. $P_n(t)=|c_n(t)|^2$.

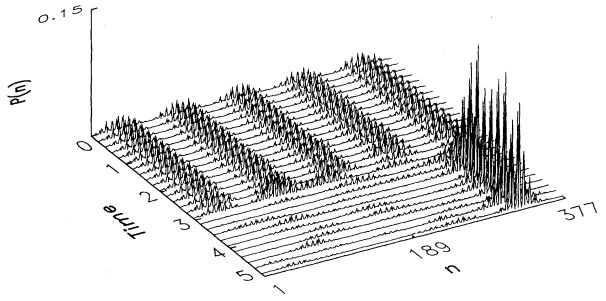


FIG. 12. Time evolution of the electronic wave function for $\varepsilon_0=1.5$, $\lambda\approx 0.21$, $N=377$, and the initial wave function being the 95th eigenstate of H_e (from the ground state up) with $E_e(0)=-1.777$. The unit of time is $t_0=t_l^2/t_e\approx 81.8t_l$.

Beyond this point, the peak is sharp and robust and the participation number seems to saturate ($P\approx 80\pm 20$). The lattice and electronic energies saturate at values comparable with the previous case [Fig. 11(a)], while $|E_{e-l}|$ is considerably larger ($E_{e-l}\approx -0.01$). Finally, in Fig. 11(c) we show a case of strongly localized polaron. A clear peak appears first for $t=t_1\approx 2t_0\approx 160t_l$ but it becomes extremely sharp at the second step, at $t=t_2\approx 10.5t_0\approx 850t_l$. Beyond this point the participation number and the various energies clearly saturate: $P\approx 22\pm 2$, $E_l\approx 0.23\pm 0.02$, $\delta E_e\approx -0.01\pm 0.01$, $E_{e-l}\approx -0.22\pm 0.03$. It is worthwhile to point out that the electronic energy initially ($t<t_1$) drops by about 0.06, slightly increases in the interval $t_1<t<t_2$, and then jumps back up by about 0.04 at the second step as a result of the strong localization. Note also that although P and the various energies have saturated for $t>t_2$, the wave function still changes with time: The satellite peak moves towards the main peak and stays at its vicinity for an extended time interval ($30t_0<t<52t_0$); however, later on (for $t>53t_0$) it moves again, this time away from the main peak toward its previous position.

Another interesting case of strongly localized polaron is shown in Fig. 12. In this case the localized polaron is formed in a single step at $t=t_1\approx 3t_0\approx 250t_l$. Beyond this point $P\approx 22\pm 5$.

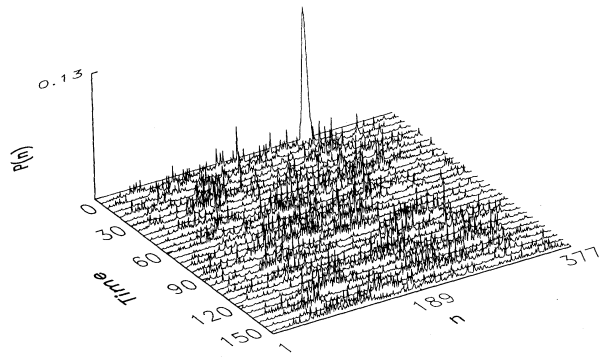


FIG. 13. Time evolution of the electronic wave function for $\varepsilon_0=1.5$, $\lambda\approx 0.024$, $N=377$, and the initial state being a Gaussian with $\sigma=3$ and $E_e(0)=-1.949$. The unit of time is $t_0=t_l^2/t_e\approx 81.8t_l$. $P_n(t)=|c_n(t)|^2$.

In Fig. 13 we show a case of large (extended) polaron with initial energy near the lower band edge and very weak coupling. The participation number shows strong fluctuations: $P\approx 120\pm 50$. The various energies E_l, δE_e, E_{e-l} after a long time ($t\approx t_1\approx 120t_0\approx 9800t_l$) seem to saturate: $E_l\approx 0.0115\pm 0.0005$, $\delta E_e\approx -0.0115\pm 0.0005$, $E_{e-l}\approx -0.0003\pm 0.0002$. Again the transfer of energy from the electron to the lattice seems to have stopped for $t>t_1$, in spite of the large difference in the effective temperatures between the electronic and the lattice degrees of freedom.

V. CONCLUDING REMARKS

The main conclusions of the present work, which may or may not be applicable to 3D random systems, are as follows.

1. As we approach the mobility edge, a smaller and smaller coupling strength is required in order to create a localized polaron. At the mobility edge an extremely weak (or even vanishingly small) coupling is sufficient to localize the electron in a lattice deformation. This behavior is summarized in Fig. 14, where the $\sqrt{\lambda}$ versus ε_0 plane is separated into regions of large or extendedlike and localized polarons by a gray area where the intermediate (I) resonancelike polarons appear. The boundaries between large and I as well as between I and local-

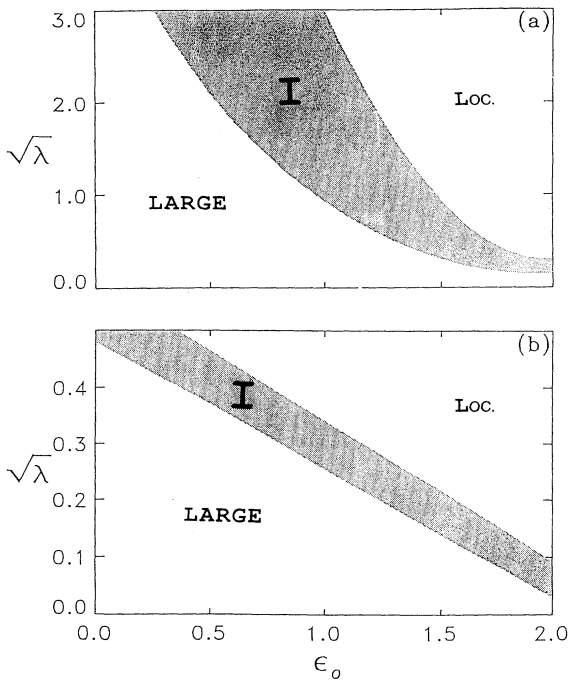


FIG. 14. Separation of the $\sqrt{\lambda}$ vs ε_0 plane into regions where large or extended intermediate resonancelike (I), and localized (Loc) polarons are expected to appear. The lower panel (b) is for initial electronic energy near the bottom of the band, while the upper one (a) for the middle of the band. The boundaries between I and Large and I and Loc regions are not sharply defined and they depend also on the shape of the initial electronic function.

ized are not well defined. Even the very existence of the I regime is questionable for an infinite system allowed to run for an infinitely long time.

If this result is of general validity, one would expect that the immediate vicinity of a mobility edge would consist of localized polaronic states. The net result would be to push the new renormalized mobility edge toward the extended region and to change the critical exponent from its unperturbed value to a much smaller one or even to make it zero (i.e., discontinuity) restoring thus the concept of a minimum metallic conductivity.[6,7] Furthermore, the localized polaronic states near the mobility edge are expected to be smoother than the unperturbed ones, possibly with higher fractal exponents.

2. Increasing the initial electronic energy from the ground state up makes the creation of a localized polaron more difficult until one reaches the center of the band, where the ability of an electron to resist trapping by lattice deformation is maximum. This is shown in Fig. 14, where the center of the band case requires much higher λ for localized polarons than the bottom of the band. This difference is more pronounced for small ε_0 (i.e., small departures for periodicity); in this case the center of the band electrons remains extended for all practical values of λ.

The formation or nonformation of localized polarons besides λ, ε_0, and the initial electronic energy, depends also—but to a lesser degree—on the shape of the initial electronic state. E.g., ss states are more difficult to localize than eigenstates of the same energy; also, uniform states or eigenstates are easier to localize than Gaussians of the same energy.

3. In the presence of strong departure from periodicity and rather strong electron-lattice interaction, and for very low initial lattice temperature, an initially highly excited electron (even one with an average energy near the center of the band) does not remain in ordinary extended band states while transferring its energy to the lattice until it reaches the bottom of the band. On the contrary, it may create novel, high-energy, long-lived localized polarons (or metastable resonancelike polarons), which interact very weakly (if at all) with the lattice. This is the regime denoted by Loc (or I) in Fig. 14(a).

4. The rate of transfer of energy from an initially highly excited electron to the ionic degrees of freedom is slowing down with increasing t and in many cases it seems that it comes eventually to a complete stop. This premature termination of relaxation does not occur only in the localized regime, where it is expected, but also in cases of extended polarons. A possible explanation for this surprising behavior is that the electron creates the polaron gradually in successive phases even in the case of large (extended) polarons. This "dressing" process leads to partial renormalization of the coupling constant between the partially formed polaron and the lattice vibration. Thus the renormalized λ is a decreasing function of time and it may even become practically zero when the polaron is fully formed, leading thus to the absence of further energy relaxation. An alternative explanation, which may be the dominant one for small λ, is that the relaxation stops as soon as the electron reaches a gap that cannot be crossed with the available phonon energies in low order of perturbation theory. Given the fragmentation of the spectrum (see Fig. 1), this explanation implies a hierarchy of relaxation times. It is worthwhile to point out also that in spite of the apparently chaotic fluctuations, memory of the initial state is retained since eigenstates are transferring energy more efficiently to the lattice than other states of the same average initial energy.

5. The time dependence of the various physical quantities exhibits an unexpected variety and richness. Many time scales appear, some of them much longer than the natural time scales of the problem (t_e, t_l, Nt_e, Nt_l). In addition the behavior of most quantities (with the exception of the total lattice energy) is very noisy.

6. The length dependence of the characteristic long-time scales and the time evolution in general of the various quantities cannot be easily classified. Some characteristic times are clearly N independent, e.g., the deeps appearing at $t=2.5t_0$, $7.5t_0$ in Fig. 10(d) for $N=377$ remain at the same instances for $N=610$. In other cases increasing the length from $N=377$ to $N=160$ smoothens out the very pronounced features, e.g., the steps at $t\approx 2t_0$ and $t\approx 6t_0$ in Fig. 6(b), to the extent that they become unrecognizable. Finally there are cases where there is an increase of some characteristic times as we change from $N=377$ to $N=610$, e.g., the characteristic deep appearing at $t\approx 0.8t_0$ in Fig. 5 appears (less pronounced) at $t\approx 1.6t_0$ for $N=610$. However, in general, if a steady state appears, it takes longer (very roughly by a factor of 2 or even more) to be reached for $N=610$ rather than for $N=377$.

7. The calculation of properly defined correlation functions as well as the analysis of the noise spectrum of various physical quantities may reveal some of the important hidden correlations that govern the behavior of the system. This study is currently under way.

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