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Localization and electron-phonon interactions in disordered systems

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PACS. 71.38+i – Polarons and electron-phonon interactions.
PACS. 71.50+t – Localized single-particle electronic states (excluding impurities).
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Abstract. – We study numerically the time evolution of the coupled system of an electron, described by a tight-binding model exhibiting metal-insulator transition, interacting with vibrational degrees of freedom. Depending on the initial energy of the electron, $E_e(0)$, its effective mass, m^*, on how close to the mobility edge it is and the strength of the electron-phonon coupling, different types of localized and extended states are formed. We find, that, in general, an increase of $E_e(0)$ decreases the ability of the system to form localized states, a large m^* does not always favor localization and polaron formation is facilitated near the mobility edge.

The interactions between electrons and disorder, and between electrons and lattice vibrations, exist in any solid-state material. Disorder modifies the motion of an electron in profound ways. The extended Bloch states develop phase incoherence and amplitude fluctuations. The sharp band edges disappear and tails of localized states emerge. In the last two decades, our understanding of a number of important issues in the field of localization has greatly advanced [1]. Electron-phonon (el-ph) interactions have also dramatic effects in some cases. It is well known, for instance, that in the case of an electron in a 1D periodic lattice, a polaronic state occurs in the presence of el-ph interaction [2]. Much less has been done to study the combined effects of disorder and el-ph interaction. It has been argued [3] that the el-ph coupling has a profound effect on the characteristic features of a disordered system. For example, it strongly enhances localization, inducing polaron formation at the so-called mobility edge, even when it is vanishingly small [3]. On the other hand, disorder also affects polaron formation. The impurities play the role of nucleation centers in the polaron formation [4]. It should be mentioned that Phillpot *et al.* [5] have studied the effects of isolated impurities in the framework of Su-Schrieffer-Heeger Hamiltonian [6]; Anderson [7] also considered the case

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of electron-intramolecular phonon coupling in the presence of a site impurity, and Bulka and Kramer[8] studied the stability of the polaron in 1D disordered systems. Most of the above theoretical work is based on the adiabatic approximation and on scaling arguments, which are simple and elegant but might possess some uncontrollable approximations. However, recently the time evolution of a combined system of an electron described by a tight-binding model interacting with vibrational degrees of freedom in 1D was studied in periodic and quasi-periodic systems [9]-[11], without imposing the adiabatic approximation. Starting with the lattice in its classical ground state and the electron in various initial states, the numerically calculated time evolutions of the system provided several types of localized and extended solutions qualitatively different from the traditional polaronic states [9], [10], as well as a remarkable recurrence phenomenon [11].

In the present letter, we examine systematically the influence of the el-ph interaction on one-electron extended states just above the so-called mobility edge, where the electronic states (in the absence of el-ph interactions) change from extended to localized. In particular, we find that indeed polaron formation is facilitated as one approaches the mobility edge [9], [10], in agreement with the scaling arguments [3]. In addition, the localization length, $\ell_{\rm c}$, decreases upon increasing the disorder for a given amount of el-ph coupling. This behavior is normal and expected. However, we have also numerically obtained results that confirm some speculative ideas based on scaling arguments concerning transport in disordered systems. We find that if the disorder is large enough to localize the system, $\ell_{\rm c}$ increases, instead of decreasing, as the el-ph coupling increases. Similar behavior is obtained for the case of strong el-ph coupling, as the disorder increases, $\ell_{\rm c}$ increases! This increase is due to phonon-assisted hopping and suggests that the mobility of a strongly localized system increases rather than decrease with temperature [12], [13]. We have also systematically studied the role of a large effective electronic mass. One might think that "heavy" electrons are easier localized than "light" electrons, but as we will show here, this is not always the case.

The Hamiltonian describing our model consists of a quasiperiodic tight-binding electronic part, $H_{\rm e}$, possessing mobility edge eigenstates (thus simulating a 3D disordered system [14]), a harmonic lattice part, $H_{\rm l}$, and a symmetrized deformation potential interaction part, $H_{\rm e\text{-}l}$ [10]. The corresponding equations of motion for the coupled electron-lattice system are

$$i\hbar \frac{{\rm d}c_n}{{\rm d}t} = [\epsilon_n + \chi(u_{n+1} - u_{n-1})]c_n - J(c_{n+1} + c_{n-1})\,, \tag{1}$$

$$M\frac{{\rm d}^2u_n}{{\rm d}t^2} = K(u_{n+1} + u_{n-1} - 2u_n) + \chi(|c_{n+1}|^2 - |c_{n-1}|^2)\,, \tag{2}$$

where c_n are the probability amplitudes to find the electron at site n ($n = 1, \ldots, N$), u_n the lattice displacements, M the atomic mass, K the interatomic force constant, J the electronic hopping matrix element, and χ the el-ph coupling strength. Notice from eq. (2) that the lattice part of the Hamiltonian is treated classically. However, not any other approximation was employed, when eqs. (1) and (2) were numerically solved. The diagonal matrix elements are $\epsilon_n = \epsilon_0 \cos(2\pi\sigma n)$, where σ is an irrational number taken as the "golden mean" $\sigma = (\sqrt{5}{+}1)/2$. Notice also that for this quasiperiodic or incommensurate choice of ϵ_n, the 1D $H_{\rm e}$ possesses a mobility edge when $\epsilon_0{=}2$. The hope is that the results of this study will be also valid, at least qualitatively, for 3D disordered systems. Throughout our calculations, we use J, M and $t_{\rm l} \equiv \sqrt{M/K}$ as the natural units of energy, mass, and time, respectively. This choice leaves us with three parameters: i) The dimensionless quantity $\hbar/Jt_{\rm l} = t_{\rm e}/t_{\rm l}$. ii) The coupling strength, χ, in units of $\sqrt{JK}$, which is the square root of $\lambda = \chi^2/KJ$, similar to the one appearing in superconductivity. iii) The disorder parameter, ϵ_0/J, which varies from 0 (periodic case) to 2 (mobility edge). The unit of length, a_0, is $\sqrt{J/K}$ in this natural system of units.

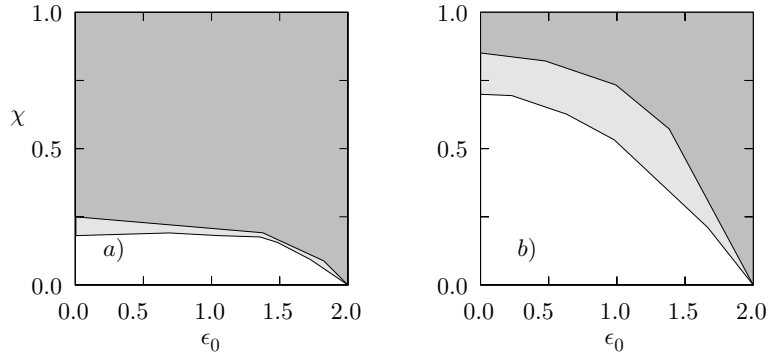

Fig. 1. – Phase diagram in the (χ, ϵ_0)-plane indicating the regions of extended and localized (shaded region) states for *a*) $t_e/t_l = 0.01224$ and *b*) $t_e/t_l = 1.0$, with the electron initially at the bottom of the band ($E_e(0) = -2.0$). Notice also the "crossover" region.

In the adiabatic and the antiadiabatic limit (*i.e.* for $M\mathrm{d}^2u_n/\mathrm{d}t^2 \approx 0$), the system of equations (1) and (2) reduces to a discrete nonlinear Schrödinger equation (DNLS) and in the continuum, one obtains the integrable nonlinear Schrödinger equation (NLS). Several versions of DNLS and the NLS have been studied intensively and their properties and solutions are known [15], since they are applicable to many different problems, including el-ph systems within the adiabatic approximation. It is well known, for example, that among other hierarchies of solutions, NLS sustains soliton solutions that are the analogs of the large polarons in the coupled el-ph system (we recover this ground-state behavior in our model in the adiabatic and weak-coupling regime [16]). However, in our approach we fully include lattice vibrations, discreteness, dispersion, el-ph coupling, nonadiabaticity and disorder. So comparison of the numerical studies of the time evolution of our coupled system with studies of DNLS and NLS is of fundamental importance.

In our numerical studies, we focus on the low-temperature case (the lattice is initially at rest and undeformed) and the electron is very close to an eigenstate of the periodic part of H_e with $E_e(0) = -2, 0$, or localized in a few sites close to the middle of the specimen, with approximately the same energies as the eigenstates above. Periodic boundary conditions are used and the time integration is performed with a fourth-order Runge-Kutta method with a step equal to 10^{-4}–$10^{-3}t_l$, such that in our simulations, energy is conserved to a relative accuracy of at least 10^{-5}. In this letter we concentrate on the time development of the participation number, $P(t) = \left[\sum_n |c_n(t)|^4\right]^{-1}$, which gives a measure of how many sites participate in the electronic wave function ($P = N$ for a uniform state and $P = 1$ for a state localized in a single site) and is proportional to the localization length, ℓ_c, for two different values of the electronic effective mass: i) $t_e/t_l = 0.01224 \ll 1$ (typical for most metals, adiabatic regime) and ii) $t_e/t_l = 1$ (narrow-band materials, nonadiabatic regime). For both cases the size of the system $N = 377$ and results for two different initial electronic configurations are presented: i) the electron very close to the uniform state at the bottom of the band with $E_e(0) = -2$ and ii) the electron localized in a single site with $E_e(0) = 0$.

The main conclusions of this work are presented in fig. 1 and 2, where the "phase diagrams" in the (χ, ϵ_0)-plane, indicating the region of extended and localized states, are shown. In fig. 1 *a*) and *b*), the results of $E_e(0) = -2$ for the small m^* ($t_e/t_l = 0.01224$) and large m^* ($t_e/t_l = 1$) are presented, respectively. In fig. 2 *a*) and *b*), the results of $E_e(0) = 0$, for the light and the heavy electron are presented, respectively. The phase diagrams describe the

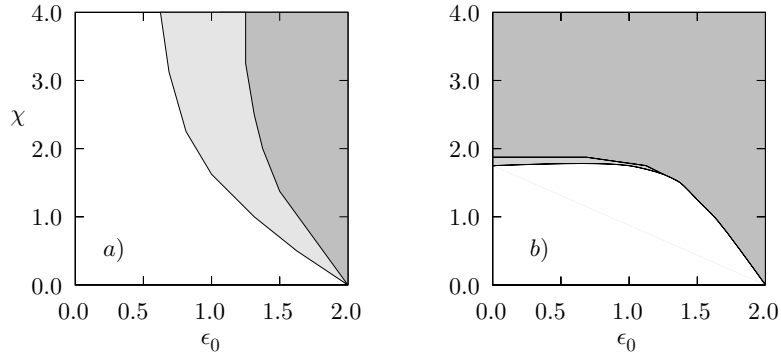

Fig. 2. – Same as in fig. 1, but with the electron initially localized in a single site, *i.e.* at the center of the band ($E_e(0) = 0$).

state reached after a time of the order of $10^5 t_l$. The boundaries ([1]) between the extended and localized regions presented in fig. 1 and 2 are not sharply defined (there is a region of "intermediate" states across the boundaries, which is significantly broad in fig. 2 *a*), for instance; the results in fig. 1 *a*) and 2 *a*) are very similar to the ones in ref. [9]). Figures 1 and 2 clearly show that for all the cases we have examined, as disorder (ϵ_0) increases, and the mobility edge ($\epsilon_0 = 2$) is approached, a localized polaron is easily formed even for extremely weak electron-phonon interaction. This general result is due to the fact that as one approaches the mobility edge from the extended side, the wave functions develop strong fluctuations and can be easily localized even with a very weak el-ph interaction. Another general feature of our studies is that increasing el-ph coupling always favors localization. However, note the case in fig. 2 *a*) for $\epsilon_0 = 0, E_e(0) = 0$ and small m^*. In this case even a very large value of the el-ph coupling ($\chi = 4$) is not enough to give localized solutions. The confinement happens easily (even for weak coupling) when the electron is initially in the ground state $E_e(0) = -2$ (fig. 1 *a*)). Figures 1 *b*) and 2 *b*) show how the "phase" diagrams change, by increasing the effective mass of the electron, for the two different initial electronic states. One might naively think that "heavy" electrons are more localized than "light" electrons. This is correct only for initially localized electrons (with $E_e(0) = 0$) as shown in fig. 2 *b*). There, increasing m^* facilitates the creation of a localized solution. Notice that even for the periodic case ($\epsilon_0 = 0$) the introduction of a large m^* gives localized polaron for $\chi \simeq 2$ (fig. 2 *b*)). For the same electron-lattice coupling ($\chi \simeq 2$) the small m^* (fig. 2 *a*)) clearly has extended solutions. However, opposite behavior is observed (fig. 2 *b*)), when the initial electronic states are extended with $E_e(0) = -2$. In this case, increasing m^* makes the creation of a localized solution more difficult. Of course, as in the case of small m^* (fig. 1 *a*), 2 *a*)), the increase of the disorder for large m^* facilitates

([1]) A clear sign of a localized state is obtained if i) P reaches a small value ($\leq N/5$), which stays the same as the size N increases. ii) The electronic wave function has one or more pronounced peaks and seems to decay away from them. iii) The change in electronic energy δE_e is positive and the interaction energy $E_{e\text{-}l}$ is larger than the lattice energy E_l. However, strong indications for extended or large polaron states are i) a large $P(\geq N/3)$ which increases with N, ii) an electronic wave function that extends over all sites of the system without a pronounced peak, and iii) a very small value of $|E_{e\text{-}l}|$ in comparison with E_l. In the "crossover" or "intermediate" region, P is roughly between $N/5$ and $N/3$, the electronic wave function has one or more peaks but it does not seem to decay as one moves away from the peaks and the values of $E_{e\text{-}l}$, E_l, and δE_e are all of the same order of magnitude. Furthermore, this "crossover" (or even some of the extended) region may disappear altogether in an infinite system and for an infinite time lapse.

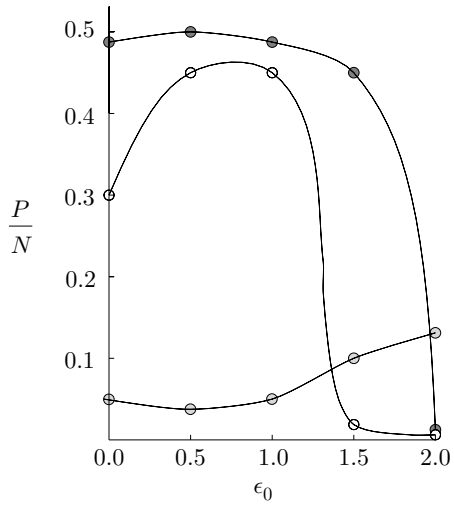

Fig. 3. – Participation number, P, *vs.* ϵ_0 for different values of χ, $E_{\rm e}(0)$, and $t_{\rm e}/t_{\rm l}$. The values for solid and open circles are $0.5, 0, 1$ and $1.0, 0, 1$, respectively, and for shaded circles $2.0, -2, 0.01224$. The size of the system $N = 377$.

localization (fig. 1 *b*) and 2 *b*)). So, the scaling arguments for polaron formation [3] are valid, as expected, for the nonadiabatic case too. This behavior can be understood by resorting to some simple qualitative arguments [16].

In fig. 3, we plot the values of the participation ratio P/N, after a time of 5000 $t_{\rm l}$, *vs.* ϵ_0, for three representative cases, where all the different behaviors of P are exhibited. The solid circles represent the case of a well-extended state in the absence of disorder with $E_{\rm e}(0) = 0$ (initially localized electron), $\chi = 0.5$, and $t_{\rm e}/t_{\rm l} = 1$. This case can be seen in fig. 2 *b*), where we keep $\chi = 0.5$ and move along the ϵ_0 axis. Notice that as disorder, ϵ_0, increases, P/N decreases as expected. The open circles represent the case of an extended state with $E_{\rm e}(0) = 0$, $\chi = 1.0$ and $t_{\rm e}/t_{\rm l} = 1$. Notice that a very interesting behavior for P/N is obtained; as ϵ_0 increases, P/N initially increases and then by further increase of ϵ_0, P/N monotonically decreases. This behavior is observed for intermediate times. For longer times, P/N for the open circles approaches that of the solid circles. Similar behavior has also been seen for extended states close to the mobility edge, by keeping the disorder constant and increasing the el-ph coupling [10]. This behavior will result in a nonmonotonic behavior of the resistivity of the system [12], [13]. Finally, if a state is strongly localized due to el-ph interaction, the introduction of disorder tends to delocalize it, *i.e.* the increase of the disorder increases the localization length, ℓ_c, instead of decreasing it, but the state still remains localized [13]. This is clearly shown in fig. 3, where the shaded circles represent the case of $E_{\rm e}(0) = -2$, $\chi = 2.0$, and $t_{\rm e}/t_{\rm l} = 0.01224$. One clearly sees that as ϵ_0 increases, P/N also increases. We attribute this increase to phonon-assisted hopping.

In conclusion, we found that: i) the character of electronic wave functions in disordered systems changes dramatically with the introduction of el-ph interaction, especially close to the mobility edge, where polaron formation is facilitated. This behavior is correct for both adiabatic and nonadiabatic electrons. ii) Close to the extended side of the mobility edge, a new physical phenomenon has been demonstrated: phonon-assisted mobility can occur in disordered systems, even in the regime of extended states, and not only in the localized regime. iii) The effects of varying the electronic effective mass, m^*, depend strongly on the initial

conditions. When the electron is initially extended at the bottom of the band, increasing m^* does not favor localization. Initially highly excited extended electronic states become localized only when the effective mass of the electron is of the order of the atomic mass. In the case of the electron initially localized in a single site, the final state becomes extended, if m^* is small, and remains localized, if m^* is large, provided χ is strong enough. In general, an increase of the initial electronic energy decreases the ability of the system to reach a localized state.

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