Dynamics in chains randomly doped with nonadiabatic impurities

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Dynamics in chains randomly doped with nonadiabatic impurities

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Abstract. We study propagation of excitations in one-dimensional tight-binding chains doped with random impurities that are classical Einstein oscillators. We find that the presence of impurities does not affect substantially the ballistic nature of the electronic propagation. Furthermore, for some oscillator masses, wave propagation is faster than that of the ordered tight-binding chain.

1. Introduction

Issues related to wave propagation in a nonlinear and disordered medium are quite important not only for theoretical reasons but also for applications [1–3]. It is known that when both nonlinearity and disorder are present new dynamical effects appear that were not anticipated when just one was present [3]. The discrete nonlinear Schrödinger (DNLS) equation provides an interesting example where the presence of disorder does not affect substantially several of its dynamical and stationary properties [3, 4]. In the present paper we will present numerical evidence showing that lifting the adiabatic hypothesis on the nature of the impurities in DNLS does not affect the dynamics substantially [5]. Furthermore, for some impurity oscillator mass values, nonadiabaticity actually *enhances* the rate of ballistic propagation to values larger than that of the ordered one dimensional tight-binding chain.

Let us consider excitation propagation in a one-dimensional lattice described in the usual tight-binding framework. The chain is coupled to a set of Einstein oscillators at random sites, forming a random binary alloy. If the oscillators are described classically, we obtain the following equations of motion [5]:

$$\mathrm{i}\frac{\mathrm{d}c_m}{\mathrm{d}t} = \epsilon_m c_m + V(c_{m+1} + c_{m-1}) + \alpha \sum_n c_m w_m \delta_{m,n} \tag{1}$$

$$M\frac{\mathrm{d}^2 w_m}{\mathrm{d}t^2} + k w_m = -\alpha |c_m|^2 \tag{2}$$

where $c_m(t)$ is the electronic probability amplitude at chain site m, $w_m(t)$ is the displacement of a local Einstein oscillator at site m, α is the local coupling coefficient between excitation and oscillator at the impurity sites, V is the nearest-neighbour wavefunction overlap, ϵ_m is

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the local site energy and M, k are the oscillator mass and spring constant respectively. The summation in equation (1) counts only the sites with impurities. The latter are typically taken from a binary random distribution with average impurity probability per site equal to 0.5.

When $M = 0$, the local oscillators adjust instantaneously to the electronic presence, and equations (1) and (2) reduce to a DNLS equation with a (random) nonlinearity parameter $\chi = \alpha^2/k$ taken from a binary distribution. This case was studied in [4] and it was found that below a nonlinearity parameter threshold, the electron did not localize despite disorder, but exhibited ballistic-like propagation. Above threshold, there was partial localization, while the untrapped part of the wavepacket escaped ballistically. In the present study, we are interested in investigating what the effect of the oscillator inertia is on the electronic propagation properties. We assume for simplicity $V = k = 1$ and $\epsilon_m = 0$, and then vary the nonlinearity parameter $\chi (= \alpha^2)$ and the oscillator inertia M and study numerically the dynamics contained in equations (1) and (2).

Placing initially the electron in an impurity site we can choose two initial-impurity site-oscillator conditions: (i) initially relaxed oscillator with $w_m(0) = -\alpha$ and $\dot{w}_m(0) = 0$ and (ii) initially undisturbed oscillator with $w_m(0) = \dot{w}_m(0) = 0$. The former oscillator initial conditions are appropriate for 'fast' oscillators with small dimensionless mass that adjust to the presence of the excitation 'instantaneously' whereas the latter are better in the large-inertia regime. For either type of initial conditions, the dynamical properties of the excitation are studied primarily through the wavepacket mean square displacement:

$$\langle m^2 \rangle = \sum_{m=-\infty}^{\infty} m^2 |c_m(t)|^2 \tag{3}$$

with normalization $\sum_{-\infty}^{\infty} |c_m(t)|^2 = 1$. For the numerics we follow [4] and use a fourth-order Runge–Kutta code, monitor the calculation accuracy through total probability conservation and eliminate boundary effects through dynamical increase of the lattice length.

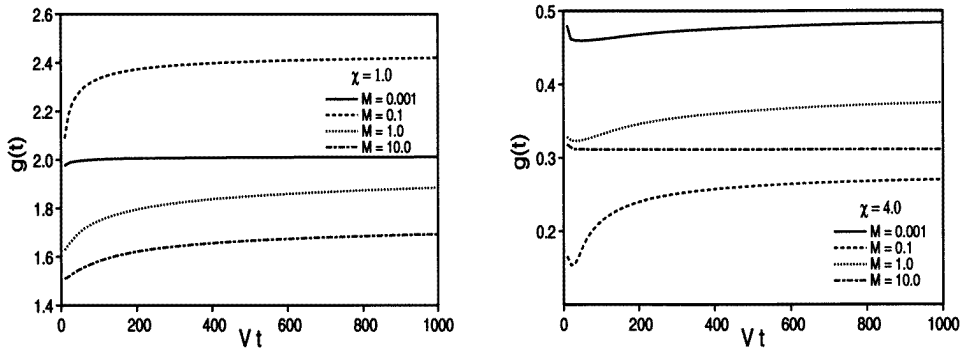

Figure 1. Rate coefficient $g(t)$ for the electronic mean square displacement as a function of time for small and large coupling and for several oscillator masses.

2. Numerical results for the propagation

We place the excitation initially at site $m = 0$ that is also an impurity site and assume the local oscillator is initially relaxed, i.e. $w_m(0) = -\sqrt{\chi}$ with zero initial velocity. In figure

1 we show the results for $g(t)$, the rate coefficient that connects the excitation mean square displacement with t^2, i.e. $\langle m(t)^2 \rangle = g(t)(Vt)^2$, as a function of time for two different values of coupling χ and various (dimensionless) oscillator masses. We note that in the perfect, ordered tight-binding chain, we have ballistic propagation with $g(t) = 2$. This ballistic nature of propagation is asymptotically valid here as well, even though we have a disordered system. In the small coupling case, i.e. for $\chi = 1.0$, ballistic motion is attained rapidly with rates close to that of the ordered case.

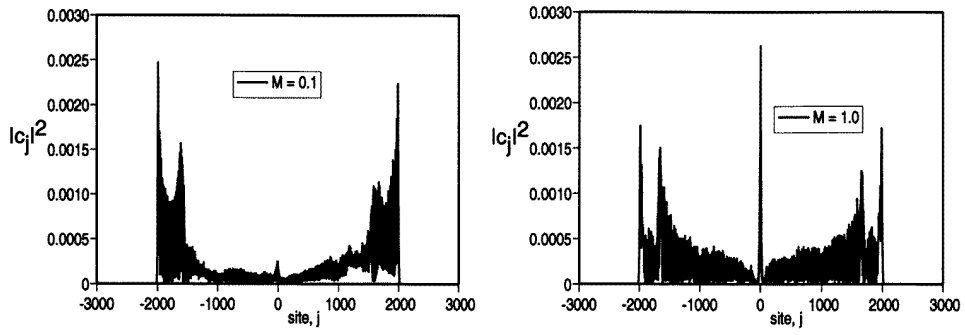

Figure 2. Electronic probability evolution portraits for different values of mass. The snap shots are taken at $Vt = 1000$, with $\chi = 1.0$.

Furthermore, we observe additionally the presence of ballistic motion with rates even larger than that of the ordered case. This happens for oscillator masses $M = 0.1$. This peculiar case will be discussed in detail in the next section. In the case of large coupling $\chi = 4.0$ we have similar ballistic evolution but with substantially reduced rates. Due to the substantial increase in coupling, part of the initial excitation probability remains in the impurity site while the untrapped portion escapes ballistically. The rate reduction is attributed to the reduction of the total wave probability that is possible to escape from the impurity site. We observe that the probability trapping effect of [5] simply results in the reduction of ballistic rate at large couplings. In figure 2 we present probability evolution portraits for different values of mass but under the same coupling. The trapped portion is clearly evident in the case of $M = 1.0$.

The case of initially unrelaxed oscillators has been also studied in detail [6]. We find similar ballistic propagation with different rates depending on the electron–oscillator coupling and oscillator masses. Since the oscillator is not initially in dynamical equilibrium with the electronic excitation we find absence of self-trapping for very large oscillator masses ($M \geqslant 10$). For masses of the order $M \sim 0.1$ we observe again ballistic effects with rates larger than the ordered tight-binding case.

3. Excitation–oscillator resonance effects

In order to study the source of the high-rate ballistic propagation observed for both types of initial conditions, in the vicinity of $\chi \approx 1.0$ and $0.1 \leqslant M \leqslant 1.0$ we focus on a single oscillator impurity coupled to the tight binding chain. Numerical results are shown in figures 3, 4 and 5. In these figures we show (a) the oscillator time evolution $w_0(t)$, (b) lattice probability profile $|c_n|^2$ at $t = 100$, (c) rate coefficient $g(t)$ and (d) excitation probability at the initial site $|c_0|^2$ for $\chi = 1$ and $M = 0.01, 0.1$ (figures 3 and 4) and $\chi = 4$,

$M = 0.1$ (figure 5). We observe that when the Einstein oscillator is excited we get high-rate ($g(t) > 2$) ballistic propagation (figure 4) while in the opposite case, i.e when the oscillator is not excited substantially, this is not true (figures 3 and 5). This oscillator excitation is accompanied with a reduction of the exciton probability in the central site, i.e. $|c_0|^2$. As a result, the high-rate ballistic exciton motion is attributed to a resonance between the local oscillator frequency and the exciton transfer rate to the nearby sites. This resonance, enhances the probability transfer rate out of the initially occupied site leading to ballistic propagation with high rate. We note that there is a range of χ and M values for which this resonance occurs. For $\chi = 1$, we obtain the most resonant case for $M = 0.2434$. We note, further, that in this mass range self-trapping occurs at $\chi \approx 3.2$, a value at which ballistic motion occurs at much smaller rates. As a result, the oscillator–exciton resonance is not related to self-trapping, and when the latter occurs, high-rate ballistic motion ceases (see figure 5).

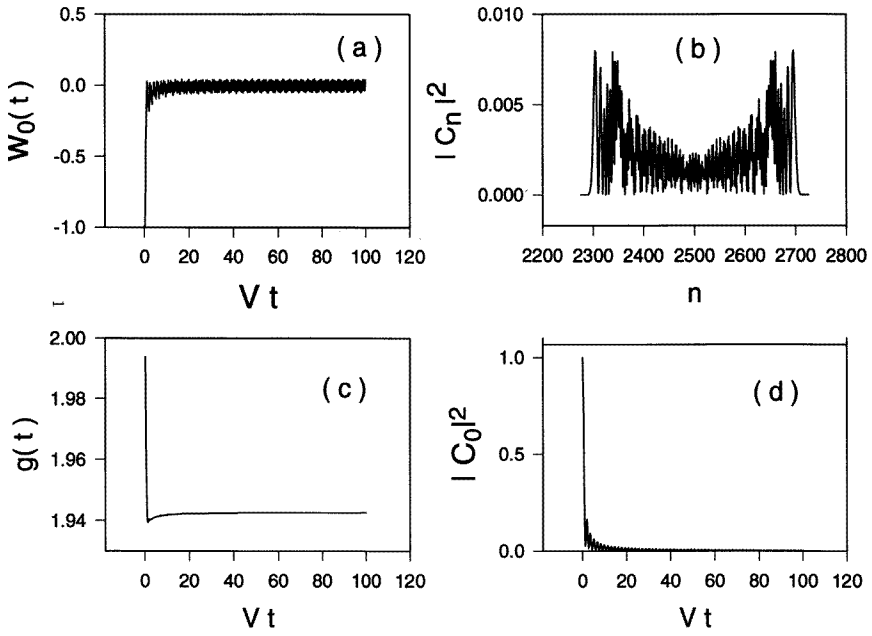

Figure 3. Single oscillator impurity with $\chi = 1.0$ and $M = 0.01$. (a) Oscillator time evolution, (b) electronic probability profile, (c) rate coefficient and (d) excitation probability at original site.

The origin of the high-rate ballistic phenomenon is intimately connected to a resonance between the exciton motion out of the initially populated site and the local classical oscillator. In the relatively small-χ regime, we can ignore the coupling between exciton and oscillator to zeroth-order. The exciton probability amplitude at the initial site will then evolve as $c_0 = J_0(2Vt)$, where J_0 is the zeroth-order Bessel function of the first kind. For $V = 1$ the timescale of the exciton oscillation out of the initial site is $\tau_e \approx T_e \approx 3.5$, where T_e is the period of the first exciton oscillation. The latter time is approximately given by the second Bessel function maximum, located between its second and third roots. The oscillator timescale, on the other hand, is $\tau_o \approx T_o = 2\pi\sqrt{M/k} \approx 6.28\sqrt{M}$. We note that when the oscillator masses are in the range of $M \approx 0.1$–0.3 the oscillator and exciton timescales

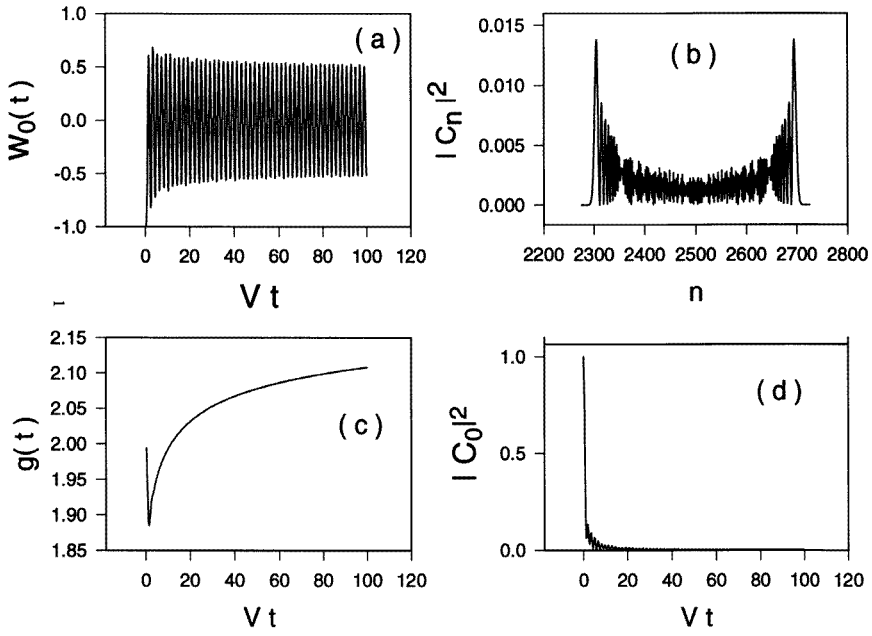

Figure 4. As figure 3 but for $\chi = 1.0$, $M = 0.1$.

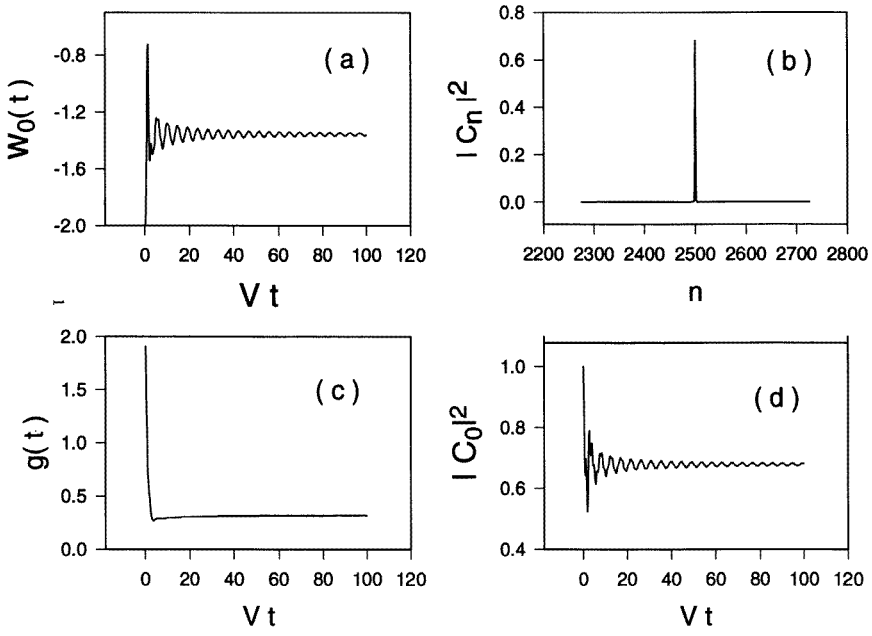

Figure 5. As figure 3 but for $\chi = 4$, $M = 0.1$.

come very close. Due to the finite value of the coupling χ a resonance occurs between the two subsystems that results in very fast ($g(t) > 2$) ballistic motion. We found numerically that the maximum transfer between the two subsystems occurs at $M = 0.2434$ for $\chi = 1.0$, leading in this case to $\tau_o \approx 3.1$. If we take into account the effective reduction of the transfer rate out of the initial site due to the finite value of χ as in [7], we find quite a good agreement between the two timescales for this most resonant case.

4. Discussion

We have studied numerically propagation of excitations in a one-dimensional tight-binding host on which we distribute randomly classical Einstein oscillators. The two systems are coupled linearly. We varied the oscillator masses as well as the coupling with the excitations and analysed primarily exciton mean square displacement. We found that for small couplings the exciton defies disorder and escapes ballistically while at large couplings ($\chi \geqslant 4$) part of the exciton gets self-trapped. The remaining untrapped portion escapes ballistically at substantially reduced rates. We found that small oscillator inertia ($0 < M < 1$) does not inhibit electronic self-trapping or the ballistic character of the propagation of the untrapped portion. For relatively small couplings, such as $\chi = 1$, when the oscillator mass becomes of the order $M \sim 0.1$ we observe ballistic motion with rates larger than the tight-binding ones. This effect is due to proximity of the two available timescales, i.e. that of the exciton transfer and the impurity oscillation. For large oscillator masses ($M \gg 1$) that are initially undisturbed by the presence of the excitation we found no self-trapping. This is in agreement with analytical results obtained for the case of one impurity [5].

Acknowledgments

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