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Self-trapping properties and recurrence phenomena in a modified discrete non-linear Schrödinger equation

G Kalosakas, G P Tsironis† and E N Economou

Research Centre of Crete, PO Box 1527, 71110 Heraklion-Crete, Greece and Department of Physics, University of Crete, 71409 Heraklion-Crete, Greece

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Abstract. We study the properties of a modified discrete non-linear Schrödinger equation (MDNLS) that arises from the coupling of an excitation to an acoustic chain. We find exact results for self-trapping in chains of two and three sites and approximate results for longer chains. We also study possible recurrence phenomena in the equation and compare our findings with those of the standard DNLS as well as the integrable DNLS. We find that dynamics in MDNLS becomes more rapidly irregular compared to the other two equations.

1. Introduction

There has been a substantial increase in interest in the study of discrete sets of non-linear dynamical equations [1]. The reason is that continuous equations, seen from the point of view of condensed matter physics, are only an approximation to the complete problem that usually respects the periodic structure of the lattice. The discrete equations on the other hand, even though more realistic, are much more challenging to tackle analytically. One of the ubiquitous discrete equations is the discrete non-linear Schrödinger equation (DNLS) [2–5]:

$$i\dot{C}_n = V(C_{n+1} + C_{n-1}) - X|C_n|^2 C_n \tag{1}$$

which arises in the general problem of polaron formation as an adiabatic equation describing the dynamics of an excitation coupled to *optical* oscillators [6]. It is the aim of the present work to analyse properties related to polaron dynamics when, contrary to the above case, the excitation is coupled to an *acoustic* chain [7, 8]. In this case and under a similar adiabatic limit one obtains the following modified discrete non-linear Schrödinger equation (MDNLS):

$$i\dot{C}_n = V(C_{n+1} + C_{n-1}) - X(|C_{n+1}|^2 + |C_{n-1}|^2 + 2|C_n|^2)C_n. \tag{2}$$

It was shown numerically in [8] that the coupled system of equations leading to a polaron shows a regime where intense recurrences occur. In this work we compare the non-linear properties of MDNLS with those of DNLS as well as the integrable DNLS (IDNLS) or the Ablowitz–Ladic equation [9] and find which of the unusual features of the coupled system are present in the MDNLS. In section 2 we study the self-trapping properties of MDNLS, in section 3 we look at its recurrence properties and in section 4 we present our conclusions.

† Also at: Computational Physics Laboratory, Department of Physics, University of North Texas, Denton, TX 76203, USA.

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2. Self-trapping properties of MDNLS

In order to compare the self-trapping properties of (2) with those of the standard DNLS of (1) we perform an analysis similar to that of Molina and Tsironis [4]. We study chains with different numbers of sites (N) using periodic and open boundary conditions. We typically consider the initial condition that places the particle at $t = 0$ at a given lattice site n_0, i.e. $C_n(t = 0) = \delta_{n,n_0}$, and compute the time-averaged probability for the particle to remain in that site, i.e. $\langle |C_{n_0}|^2 \rangle$. We consider both positive and negative V, taken to be $V = \pm 1$, and the non-linearity parameter X takes different positive values.

2.1. Exact results

For the dimer ($N = 2$) and periodic trimer ($N = 3$) case we can find solutions of (2) in closed form. We first write (2) using the density matrix $\rho_{m,n} = C_m C_n^*$. We find that for these two cases the equations of motion for $\rho_{m,n}$ are exactly the same as the corresponding ones that arise from DNLS. Consequently, for the dimer case we have the same analytical solution found in [3] for the DNLS dimer, where the critical value of X for self-trapping is $X_{st} = 4|V|$ and occurs for both $V = \pm 1$. Similarly for the periodic trimer we have the same solution as in [4] for the localized initial condition that gives $X_{st} = -6V$ (there is abrupt transition only for $V = -1$).

This accidental event, where systems obeying different non-linear equations have exactly the same time evolution, occurs only in these two cases, as can be seen from the equations for the time dependence of $\rho_{m,n}$. From (2) we have for every $m, n = 1, \ldots, N$:

$$i\frac{d\rho_{m,n}}{dt} = V(\rho_{m+1,n} + \rho_{m-1,n} - \rho_{m,n+1} - \rho_{m,n-1}) - X(\rho_{m+1,m+1} + \rho_{m-1,m-1} + 2\rho_{m,m} - \rho_{n+1,n+1} - \rho_{n-1,n-1} - 2\rho_{n,n})\rho_{m,n}. \quad (3)$$

Comparing with the corresponding equation for the DNLS case (see (2) in [3]) we see that the equations differ in the term

$$-X(\rho_{m+1,m+1} + \rho_{m-1,m-1} + \rho_{m,m} - \rho_{n+1,n+1} - \rho_{n-1,n-1} - \rho_{n,n})\rho_{m,n}$$

which vanishes for all m, n only in the dimer case and periodic trimer case.

Solutions in closed form can be found also for the open trimer case with the initial condition $C_2(t = 0) = 1$. In this case using the symmetry of the problem we obtain a closed-form equation for $|C_2(t)|^2 = \rho_{2,2}$ i.e. $\frac{1}{2}\dot{\rho}_{2,2}^2 + W(\rho_{2,2}) = 0$, where

$$W(\rho) = V^2[\tfrac{1}{8}a^2\rho^4 + (4 - \tfrac{1}{4}a^2)\rho^2 - 4\rho + \tfrac{1}{8}a^2] \quad (4)$$

with $a = X/V$. We have $W(\rho = 1) = 0$.

In order for a self-trapping transition to occur the potential $W(\rho)$ must develop a double root in the range $0 < \rho < 1$, or equivalently there should be a common real root for the equations $W(\rho) = 0$ and $dW/d\rho = 0$. This is not true for the function $W(\rho)$ of (4). We note that in the corresponding DNLS open trimer case there is also absence of an abrupt transition while the equation for $\rho_{2,2}$ is different from (4) [10].

2.2. Numerical results

For the open trimer case with initial condition $C_1(t=0)=1, n_0=1$ and for chains with a larger number of sites (N from 4 to 101) we compute numerically the time-averaged probability for a return to the initial site, i.e. $\langle |C_{n_0}|^2 \rangle$. For open chains we take two different initial conditions $C_n(t=0)=\delta_{n,n_0}$ with (a) $n_0=1$ and (b) $n_0=N/2$ for N even or $n_0=(N+1)/2$ for N odd. For simplicity, the first case will be referred to as the initial condition at site 1 and the second as the initial condition at site $N/2$. Summarizing our findings, we have the following.

(i) For periodic boundary conditions and N even we have the same time evolution for both values of $V=\pm 1$. For N odd the results are different for $V=+1$ and $V=-1$. There is no abrupt transition for $N=3$ or $N=5$ and $V=+1$, although there is one for $V=-1$. For other odd-N lattices the self-trapping transition appears at the same critical X_{st} for both $V=\pm 1$ (except for the case $N=15$ that there is a small difference between two opposite V values). We observe that for periodic chains the critical non-linearity X_{st} for a self-trapping transition begins from $X=6$ and decreases for larger N until the limiting value $X=1.85$ (see figure 1).

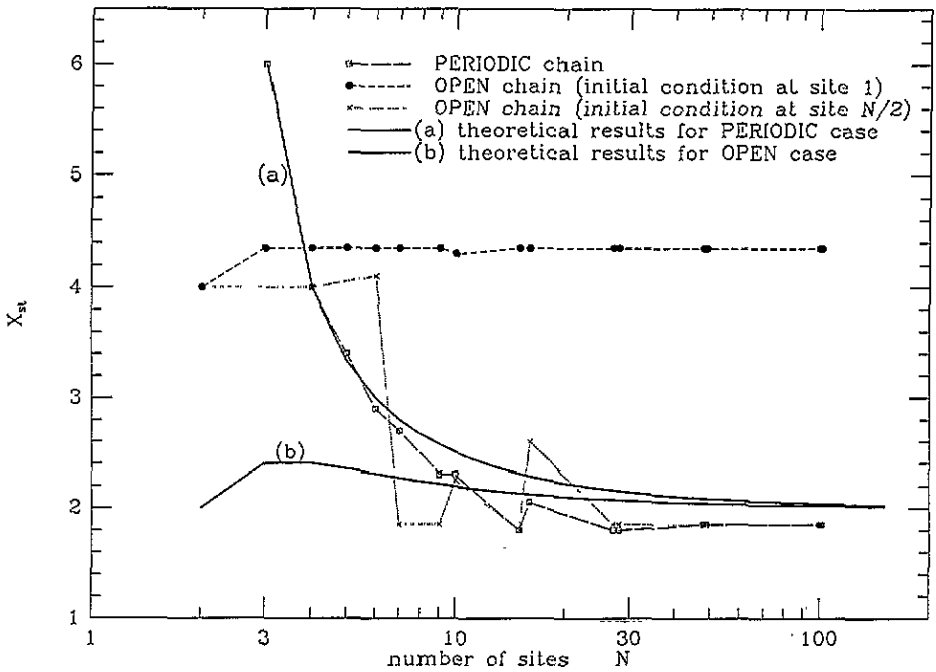

Figure 1. Critical value of X, for the self-trapping transition as a function of the number of sites N for (i) a periodic chain (squares), (ii) an open chain with a localized initial condition at site 1 (bullets) and (iii) an open chain with initial condition at site $N/2$ (crosses). In all cases $V=-1$. The full line is a guide for the eye. Also we have plotted results (full curves) obtained from theoretical arguments: (a) for the periodic case and (b) for the open case.

(ii) For open chains and initial conditions at site 1 we have the same time evolution for both values of $V=\pm 1$ and both even and odd N values. With the exception of the dimer case ($X_{st}=4$) the critical value for self-trapping does not seem to depend on N being approximately equal to $X_{st}=4.35$ (see figure 1).

(iii) For open boundary conditions and the initial condition at site $N/2$ we study the case $V = -1$. Here the critical value is about 4 until $N = 6$ (for $N = 3$ and $N = 5$ there is no abrupt transition), and for N up to 7 the X_{st} is about 2. For very large N the X_{st} reach the limiting value 1.85, as expected, since for $N \gg 1$ the results from an open chain with initial condition at the site $N/2$ must coincide with those of the periodic case (see figure 1).

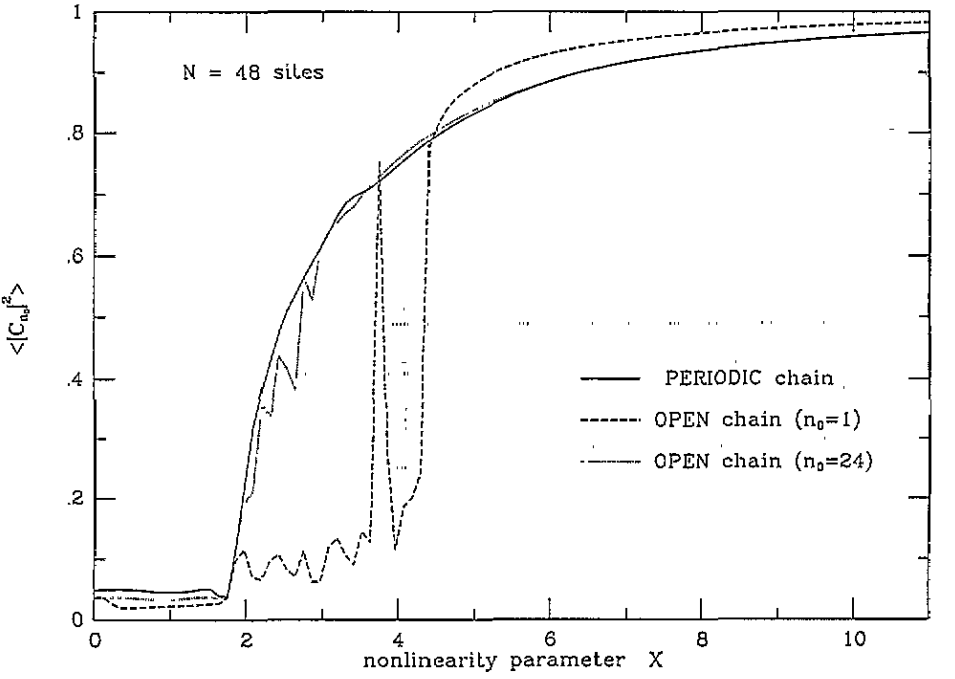

Figure 2. Time-averaged probability $\langle |C_{n_0}|^2 \rangle$ for an initially occupied site n_0 as a function of the non-linearity parameter X for a chain with $N = 48$ sites and (i) periodic boundary conditions (full curve), (ii) open boundary conditions and $n_0 = 1$ (broken curve) and (iii) open boundary conditions and $n_0 = 24$ (dotted curve). In all cases $V = -1$.

In figure 1 we summarize all the results for cases (i), (ii) and (iii) for $V = -1$. In figure 2 we plot $\langle |C_{n_0}|^2 \rangle$ as a function of X for $N = 48$ ($V = -1$). We observe the presence of irregular fluctuations prior to the trapped regime in the case of an open chain and initial conditions starting from site $n_0 = 1$. This is true for other values of N as well. Furthermore, the very strong peak at $X = 3.74$ appears in a systematic way at the same position, almost for all different N. For the periodic case and smaller N we also observe similar fluctuations, but with smaller strength and width. These features are similar to those observed for DNLS [4]. We see that MDNLS shares common features with the standard DNLS. We note, however, that the systematic strong peak at a certain position before the self-trapping transition is characteristic only of MDNLS. Another important difference between two non-linear equations is that in the periodic case for large N the self-trapping transition occurs for a smaller value of X for MDNLS than for DNLS. This value is about 1.85 for (2) and 4.00 for DNLS [4]. For the case of open chains and initial conditions at site 1 we have X_{st} equal to 4.35 in MDNLS and 4.00 in DNLS respectively.

2.3. Comparison with theoretical estimates for self-trapping

Equation (2) can be derived from the following Hamiltonian:

$$H = V\sum_m (C_m C_{m+1}^* + C_m^* C_{m+1}) - X\sum_m (|C_{m+1}|^2|C_{m+2}|^2 + |C_m|^4) \tag{5}$$

using the equations of motion $\dot{C}_n = \{H, C_n\}$ with $\{C_m, C_n^*\} = i\delta_{m,n}$, $\{C_m, C_n\} = 0 = \{C_m^*, C_n^*\}$, where $\{,\}$ are the standard Poisson brackets. Bernstein and co-workers [11] suggested a simple way of using the Hamiltonian for DNLS as well as conservation of energy for estimating the location of the self-trapping transition occurring in a chain with a finite number of sites N. Their calculations for DNLS are consistent with the numerical findings and other analytical results. In order to repeat their calculations for MDNLS we need the single-site energy H_{ss} (the value of H in the case that all the probability is concentrated on a single site, i.e. $C_i = 1$ for some i and $C_j = 0$ for $j \neq i$) and the equipartioned-state energy H_{eq} (the value of H in the case that $C_i = \sqrt{1/N}$ for all i). In [11] it was assumed that equating H_{ss} with H_{eq} and solving for X we obtain an estimate for the critical value of the non-linearity parameter at the self-trapping transition. In our case we have from (5) that $H_{ss} = -X$ and for an open chain we obtain

$$H_{eq} = 2V\frac{N-1}{N} - \frac{2X}{N} + \frac{2X}{N^2}.$$

Using the condition $H_{ss} = H_{eq}$ leads to the following critical X:

$$X_{st} = -2V\frac{N(N-1)}{(N-1)^2+1}. \tag{6}$$

For the periodic chain, on the other hand, $H_{eq} = 2V - 2X/N$ and the condition $H_{ss} = H_{eq}$ leads to

$$X_{st} = -2V\frac{N}{N-2}. \tag{7}$$

In figure 1 we plot the relations (6) and (7) respectively, along with numerical results for comparison. We note that there is very good agreement in the periodic chain case. For open chains there is agreement for $N > 6$ if we take initial conditions at site $N/2$.

3. Recurrence phenomena

The occurrence of recurrence phenomena in the solutions of non-linear differential equations has been well known since the work of Fermi and co-workers, who studied numerically vibrations in non-linear lattices [12]. Similar phenomena have been observed both numerically and experimentally in the continuum NLS equation

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + \chi|u|^2 u = 0$$

resulting from a Benjamin–Feir instability [13]. A behaviour of the same type has been observed in the context of the more complicated coupled electron–phonon system described in [8]. It is interesting to find out whether the recurrence observed reflects properties

of the MDNLS or if it is inherent in the electron–phonon system. For this purpose we study dynamical properties of the MDNLS for different initial conditions that might lead to recurrence behaviour, and compare its behaviour with two other non-linear equations, i.e. the DNLS and the integrable DNLS (IDNLS), or Ablowitz–Ladic equation [9, 14]:

$$i\dot{C}_n = V(C_{n+1} + C_{n-1}) - X|C_n|^2(C_{n+1} + C_{n-1}). \tag{8}$$

Equation (8) is completely integrable [9]. All three equations (DNLS, MDNLS, IDNLS) are different discrete versions of continuum NLS equation. In order to compare the three discrete versions of NLS we assume an initial state that is an eigenstate of the tight-binding part (i.e. the part obtained for $X = 0$). The initial condition has the form $\mathrm{Re}\big(C_n(t=0)\big) = \sqrt{2/N}\cos(kn)$ and $\mathrm{Im}\big(C_n(t=0)\big) = 0$, where N is the number of sites and k is the wavenumber. We input this initial condition, follow the time evolution for all probability amplitudes and calculate the participation number $P(t) = 1/(\sum_n |C_n(t)|^4)$, which is very sensitive to wavefunction changes. The quantity P is an indicator of the localization of the wavepacket. When $P = 1$, for instance, the packet is completely confined in a single site (i.e. $|C_n|^2 = \delta_{n,n_0}$) whereas for a completely delocalized state (i.e. $|C_n|^2 = 1/N$, $\forall n$) we have $P = N$.

3.1. Dependence on the non-linearity parameter X

In the numerical evaluation of $P(t)$ we assume that $V = -1$ and a lattice with $N = 300$ sites. For each wavenumber k considered we vary the non-linearity coefficient X in the range 0–5. The wavenumber k has been taken equal to $\pi/3$ (which is the value for which the coupled electron–phonon system exhibits recurrence behaviour), $\pi/6$ or $\pi/3.3333$. Qualitatively the behaviour of $P(t)$ is the same for DNLS and MDNLS. After an initial period of almost perfect periodicity in time this behaviour terminates and $P(t)$ becomes aperiodic (figures 3 and 4). The integrable equation IDNLS behaves in a similar fashion except that after the termination of the initial periodic behaviour there are still periodic features in the evolution (see figure 4(*b*)). The characteristic time t_0 for the end of the initial period is not the same in the three equations and additionally depends on the non-linearity parameter.

Changing the value of the non-linearity parameter X has the following two effects on $P(t)$. (i) It affects the amplitude of the periodic oscillations that become larger for higher values of X. Note that for $X = 0$ the amplitude of the oscillations vanishes since we have an exact eigenstate and there is no time dependence in the participation number. (ii) It affects the characteristic time t_0 that signals the destruction of the initial periodic behaviour. For larger values of X the characteristic time t_0 becomes smaller and the periodic phenomena disappear earlier (see figures 3(*a*) and 3(*b*)). All three equations share qualitatively this dependence on X. We note, however, that t_0 is generally smaller for the MDNLS than for the other two equations (see figure 3(*b*) and figure 4) leading to the conclusion that MDNLS has more chaotic features than the other two equations. Finally, we should point out that this initial periodic behaviour is observed only for wavenumber k that correspond to eigenstates of the tight-binding part of the equations. Even for small perturbations from these exact eigenstates the periodic features disappear.

3.2. Dependence on the length of the lattice N

To find the dependence of the initial periodic behaviour on the length we considered two chains with $N = 40$ and 300 and examined the time evolution of a common initial eigenstate. For IDNLS and $N = 40$ although the system seems to acquire chaotic behaviour, suddenly

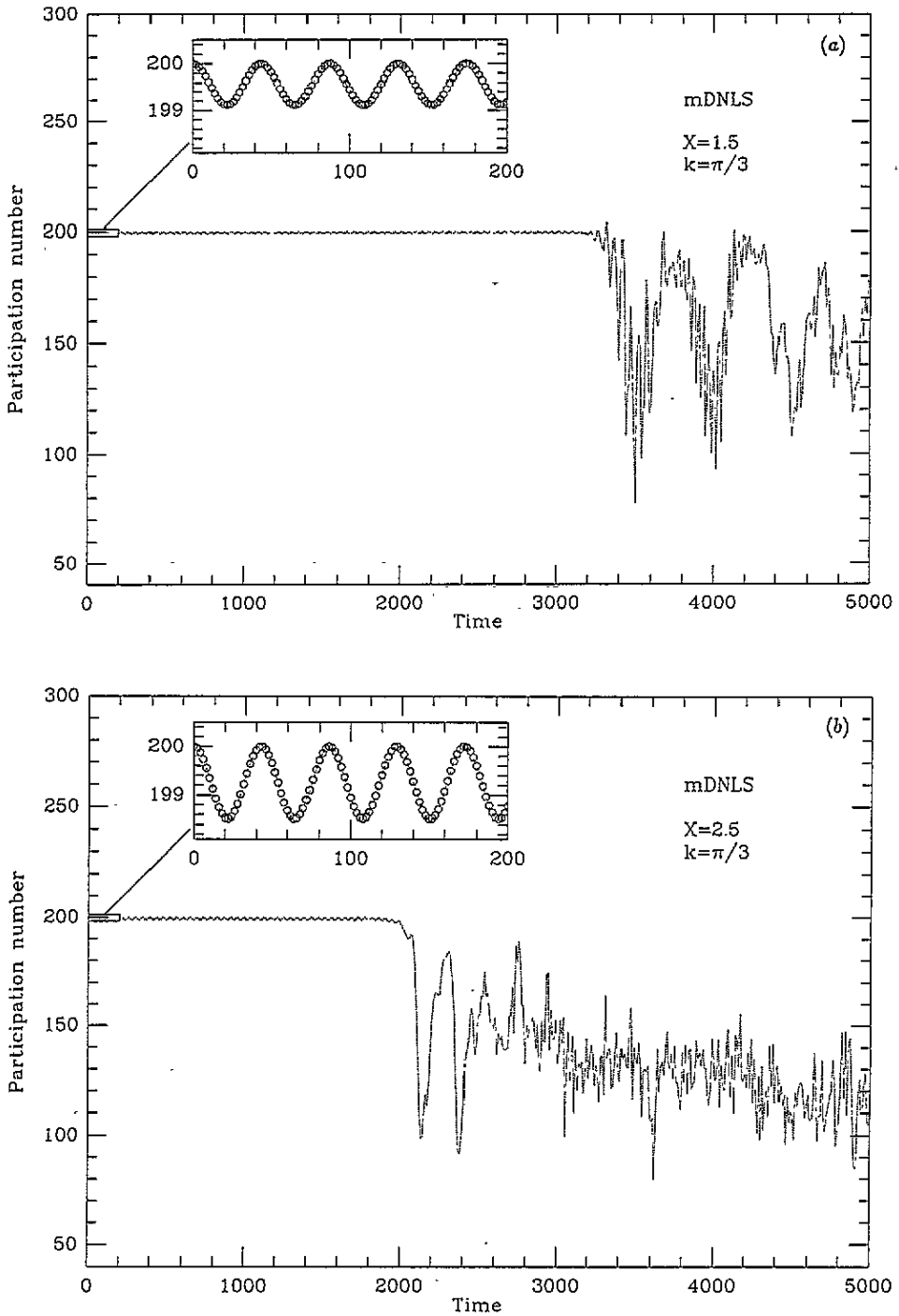

Figure 3. (*a*) Time evolution of participation number $P(t)$ for the MDNLS equation. We have $X = 1.54$, $k = \pi/3$, $N = 300$ sites and $V = -1$. (*b*) Same as (*a*) with $X = 2.5$, $k = \pi/3$, $N = 300$ sites and $V = -1$.

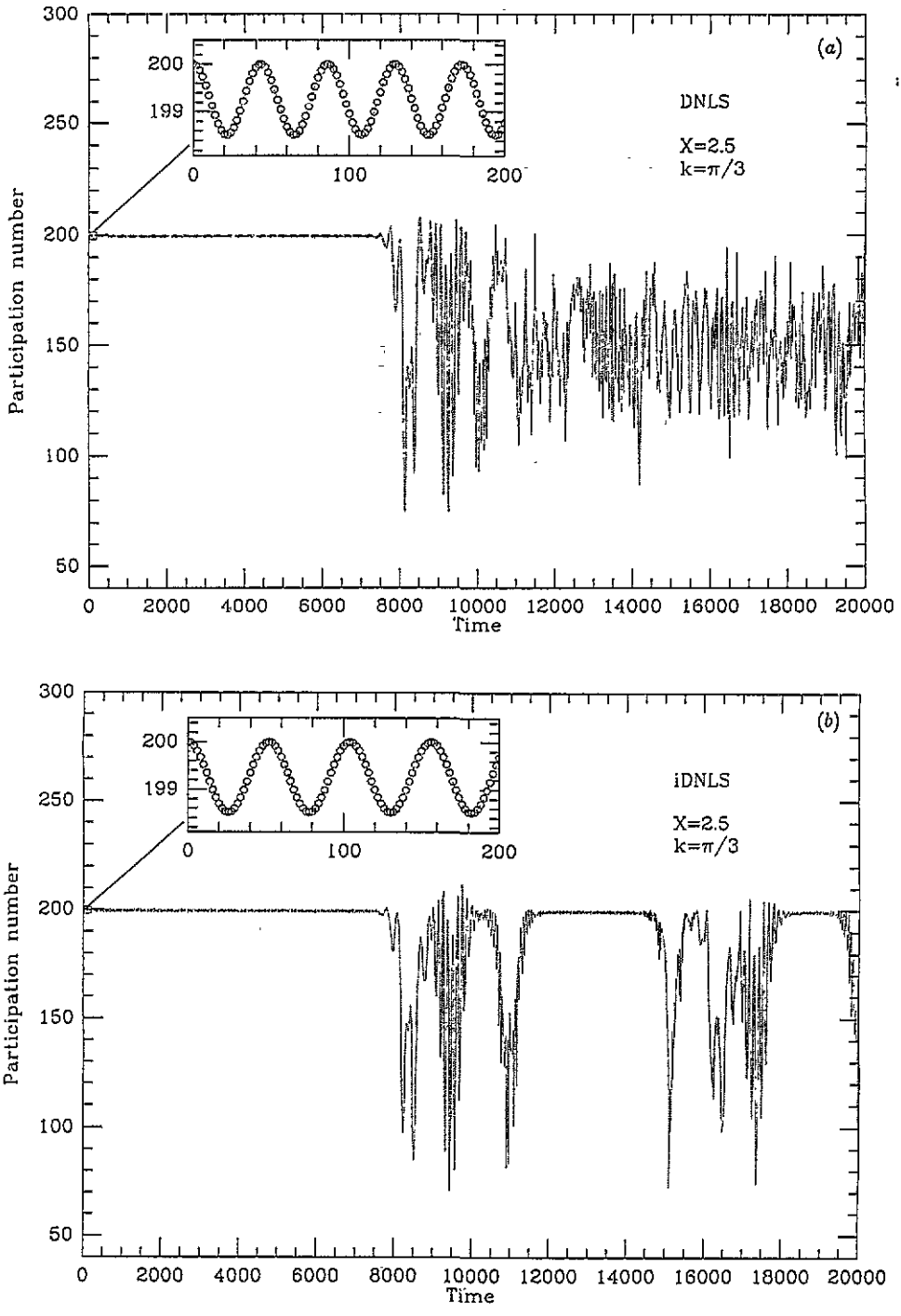

Figure 4. (*a*) Time evolution of participation number $P(t)$ for the DNLS equation. We have $X = 2.5$, $k = \pi/3$, $N = 300$ sites and $V = -1$. (*b*) Same as (*a*) for the integrable IDNLS equation. We have $X = 2.5$, $k = \pi/3$, $N = 300$ sites and $V = -1$.

periodicity is re-established and all of this phenomenon is repeated with surprising regularity. This behaviour reveals a tendency of the system to form a localized structure (such as a 'soliton'). The DNLS appears more chaotic than IDNLS for $N = 40$, whereas for $N = 300$ the behaviour of the two is quite similar, as expected since DNLS converges to the analytical solution for large chains [4, 15]. For the MDNLS case we find that, for $N = 300$, the initially periodic behaviour disappears faster than in DNLS and IDNLS. For $N = 40$ the periodicity does not even have time to appear.

4. Conclusions

In the present work we presented an analytical and a numerical study of a modified discrete non-linear Schrödinger equation and compared it with two other well known equations, i.e. DNLS and IDNLS. The MDNLS occurs as a special limit in the dynamics of an electron coupled to an acoustic chain with a symmetric coupling [7, 8]. The motivation for the present work is the recurrence phenomena found in [8] in the context of the complete coupled problem. We applied well known approaches from the study of DNLS [3,4,11] and analysed the dynamical features of MDNLS. We found that in the case of a dimer and periodic trimer the resulting equations are identical to those of DNLS, resulting in an identical evolution. We also found that for the long periodic case the self-trapping transition occurs for smaller values of non-linearity coefficient compared to the corresponding ones of DNLS. For chains of various lengths we observe initially periodic behaviour that ceases to exist after an initial period that depends on the value of the non-linearity parameter. The behaviour of MDNLS appears to have more irregular features than the DNLS and IDNLS equations. These features consist of a much faster transition to a non-periodic regime (figures 3 and 4) for any number of sites. We conclude that the recurrence phenomena observed in the coupled electron–acoustic lattice system [8] cannot be attributed to the MDNLS part, but are genuine effects of the interaction with the acoustic chain. It is worthwhile to point out that those recurrence phenomena were sustained for times of the order of 10^7 (in our units of $\hbar = 1$, $V = 1$), i.e. many orders of magnitude larger than the initial periodic behaviour exhibited in the present results. It would be interesting to look for recurrences of the type seen in [8] in the context of DNLS as well. In this case, one would have to study the interaction of the electron with an optical chain of the Holstein type [16].

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