Localized states due to the coupling of exciton with the coupled lattice oscillators

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Abstract

Discrete nonlinear Schrödinger equation (DNLS) of the form, $i \frac{dC_n}{dt} = C_{n+1} + C_{n-1} + \chi_n |C_{n+1}|^2 + |C_{n-1}|^2 - 2|C_n|^2 C_n$ is used to study the formation of stationary localized states in one dimensional system due to a single as well as a dimeric nonlinear impurity. The fully nonlinear chain is also considered. The stability of the states and its connection with the nonlinear strength is presented. Results are compared with those obtained from other DNLS. It is found that the DNLS used in this paper has more impact in the formation of stationary localized states.

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I. INTRODUCTION

It is well known that the transport properties of a system is directly related with the formation of localized states in the system. Localized states appear due to the presence of impurity or disorder (which breaks the translational symmetry) in the system \[1\]. There has been studies on the formation of localized states due to linear impurities in various systems \[1\]. On the other hand, only a few look into the formation of localized states due to nonlinear impurities. The discrete nonlinear Schrödinger equation, used to study the formation of stationary localized (SL) states \[2–13\] is given by

\[
i \frac{dC_n}{dt} = \epsilon_n C_n + V(C_{n+1} + C_{n-1}) - \chi_n |C_n|^p C_n,
\]

(1)

here \(C_n\) is the probability amplitude of the particle (exciton) to be at the site \(n\), \(\epsilon_n\) and \(\chi_n\) are the static site energy and the nonlinear strength at site \(n\) respectively and \(V\) is the nearest neighbor hopping element. The nonlinear term \(|C_n|^p C_n\) arises due to the interaction of the exciton with the lattice vibration \[14,15\]. The above eq. (1), has been used to study the formation of SL states in one dimensional chain as well as in Cayley tree with single and dimeric nonlinear impurities \[2,3,9–11\]. For the case of a perfectly nonlinear chain where \(\chi_n = \chi\), it has been shown that SL states are possible even though the translational symmetry of the system is preserved \[1,3,4,13\]. These results were remarkably different when compared with that of the corresponding systems with linear impurities.

The equation (1) has been derived with the assumption that the lattice oscillators in the system are local and oscillate independently. A natural question to ask is, what happens to the formation of SL states when the oscillators in the lattice are occupied with their nearest neighbors. In this case the discrete nonlinear Schrödinger equation takes the form

\[
i \frac{dC_n}{dt} = \epsilon_n C_n + V(C_{n+1} + C_{n-1}) - \chi_n (|C_{n+1}|^2 + |C_{n-1}|^2 - 2|C_n|^2) C_n
\]

(2)

where \(C_n\), \(\epsilon_n\), \(V\) and \(\chi_n\) carries the same meaning as in eq. (1). We notice that the eq. (2) has more nonlinear terms compared to the eq. (1). To the best of our knowledge, this
equation has not been used to study the formation of SL states even though eq. (2) is more important in condensed matter physics. Our intention is to look for the formation of SL states in one dimensional system due to the presence of nonlinear impurities (as described by eq. (2)) and further to compare the results with those obtained from eq. (1) and to see which one has more impact in the formation of SL states.

The organization of the paper is as follows. In sec. II we discuss the effect on the formation of SL states due to a single impurity (i.e. \( \chi_n = \chi(\delta_n,0) \)). In sec. III we consider the case of dimeric impurity (i.e. \( \chi_n = \chi(\delta_n,0+\delta_n,1) \)) and in sec IV we consider the perfectly nonlinear chain. In sec V we discuss about the stability of the SL states. Finally in sec. VI we summarize our findings.

## II. SINGLE NONLINEAR IMPURITY

Consider the system of a one dimensional chain with a nonlinear impurity at the central site. The time evolution of an exciton in the system is governed by eq.(2) with \( \chi_n = \chi_{\delta_n,0} \). The Hamiltonian which can produce the equation of motion for the exciton in the system is given by

\[
H = \sum_n (C_n^* C_{n+1} + C_n C_{n+1}^*) - \frac{\chi}{2} [ |C_1|^2 + |C_{-1}|^2 - 2 |C_0|^2 ] |C_0|^2.
\]  

As \( \sum_n |C_n|^2 \) is a constant of motion, we suitably renormalized so that \( \sum_n |C_n|^2 = 1 \). We call it normalization constant. Therefore, \( |C_n|^2 \) can be treated as the probability for the exciton to be at site \( n \). Since we are interested in finding the stationary localized states, we consider the ansatz

\[
C_n = \phi_n exp(-iEt); \quad \phi_n = \phi_0 |n|
\]  

where \( 0 < \eta < 1 \) and \( \eta \) can be asymptotically defined as \( \eta = \frac{|E| - \sqrt{E^2 - 4}}{2} \). \( E \) is the energy of the localized state which appears outside the host band. Since in a one dimensional system, states appearing outside the host band are exponentially localized, the ansatz (in eq. (4)) is
justified as can also be readily derived from the Greens function analysis \([9,10]\). Substituting the ansatz in the normalization condition we get
\[
|\phi_0|^2 = \frac{1 - \eta^2}{1 + \eta^2}.
\] (5)

Direct substitution for \(\phi_0, \phi_n\) and hence \(C_n\) in terms of \(\eta\) in eq. (3), yields an effective Hamiltonian,
\[
H_{\text{eff}} = \frac{4\eta}{1 + \eta^2} + \frac{\chi (1 - \eta^2)^3}{(1 + \eta^2)^2}.
\] (6)

The fixed point solutions of the reduced dynamical system described by \(H_{\text{eff}}\) will give the values of \(\eta\) (which correspond to the localized state solutions) \([8]\). Note that the effective Hamiltonian is a function of only one dynamical variable, namely, \(\eta\) as \(\chi\) is constant. Thus fixed point solutions are readily obtained from the condition \(\partial H_{\text{eff}} / \partial \eta = 0\), i.e.,
\[
\frac{4}{\chi} = \frac{\eta (1 - \eta^2)(10 + 2\eta^2)}{(1 + \eta^2)} = f(\eta).
\] (7)

Thus the different values of \(\eta \in [0,1]\) satisfying the eq. (7) will give the possible SL states for a given value of \(\chi\). It is clear from the expression for \(f(\eta)\) that \(f(\eta) \to 0\) as \(\eta \to 0\) and \(\eta \to 1\). Therefore it is expected that \(f(\eta)\) will have at least one maximum, which is indeed the case as can be seen from Fig. (1) where \(f(\eta)\) is plotted as a function of \(\eta\). Notice that there will be no graphical solution if \(\frac{4}{\chi} > f(\eta_{\text{max}})\), one solution if \(\frac{4}{\chi} = f(\eta_{\text{max}})\) and two solutions if \(\frac{4}{\chi} < f(\eta_{\text{max}})\). Thus there is a critical value of \(\chi\), say, \(\chi_{\text{cr}}\) below which no localized states are possible and is given by
\[
\chi_{\text{cr}} = \frac{\eta_{\text{max}}(1 - \eta_{\text{max}}^2)(10 + 2\eta_{\text{max}}^2)}{4(1 + \eta_{\text{max}}^2)} = 1.2696.
\] (8)

Thus for \(\chi=1.2696\), we get one SL state and two for \(\chi > 1.2696\). For a system described by eq. (1) (with \(\sigma=2\)), it has been shown in ref. \([3,9]\) that the corresponding critical value for \(\chi\) is 2. Also the maximum number of SL states possible was 1. Thus we see that the nonlinearity arising in eq. (2) reduces the critical strength and produces more number of SL states. Hence, the eq. (2) is indeed more effective in the formation of SL states.
III. DIMERIC NONLINEAR IMPURITY

We consider the case where the one dimensional lattice has two nonlinear impurities at site 0 and 1 respectively, i.e., $\chi(\delta_{n,0} + \delta_{n,1})$. As in the case of single impurity, it is easily verified that the Hamiltonian for the system is given by eq. (2) with $\chi$ as defined above. For stationarity condition we assume that $C_n = \phi_n e^{iEt}$. Furthermore, for localized states we assume the following form for $\phi_n$.

$$\phi_n = [\text{sgn}(E)\eta]^{n-1}\phi_1; \quad n \geq 1$$

and

$$\phi_{-|n|} = [\text{sgn}(E)\eta]^{|n|}\phi_0; \quad n \leq 0$$

with $\eta$ as defined earlier. The ansatz is justified as those states which appear outside the host band are exponentially localized (which can be derived exactly from the Greens function analysis [1]). Three different possibilities arise. (i) $\phi_1 = \phi_0$ (symmetric case), (ii) $\phi_1 = -\phi_0$ (antisymmetric case) and (iii) $\phi_1 \neq \phi_0$ (asymmetric case). It is possible to encompass all the different cases by introducing a variable $\beta = \phi_0/\phi_1$. The value of $\beta$ is confined between 1 and -1 if $|\phi_0| \leq \phi_1$. Else we inverse the definition of $\beta$. $\beta = 1, -1, \text{and } \neq 1$ correspond to the symmetric, antisymmetric and the asymmetric state respectively. Substituting the ansatz as well as the definition of $\beta$ in the normalization condition, $\sum_{-\infty}^{\infty} |C_n|^2 = 1$ we get

$$|\phi_0|^2 = \frac{1 - \eta^2}{1 + \beta^2}$$

and the reduced Hamiltonian

$$H_{\text{eff}} = 2\beta \frac{1 - \eta^2}{1 + \beta^2} + 2\text{sgn}(E)\eta - \frac{\chi(1 - \eta^2)^3}{2(1 + \beta^2)}.$$  \hspace{1cm} (11)

If $\beta = \pm 1$ we get,

$$H_{\text{eff}}^{\pm} = \mp 2\eta + 2\text{sgn}(E) + 3\chi \eta \frac{(1 - \eta^2)^2}{2}.$$  \hspace{1cm} (12)

Here '+' sign corresponds to the symmetric case and '-' sign corresponds to the antisymmetric case. The number of fixed point solutions of the reduced dynamical system described by $H_{\text{eff}}$ gives the the possible number of SL states. The fixed point solutions satisfy the equation,
From eq. (13) it is clear that there exists two critical values of $\chi$ namely, 0.7149 and 1.6525. There is no SL state for $\chi < 0.7149$, one symmetric SL state at $\chi = 0.7149$, two symmetric SL states for $0.7149 < \chi < 1.6525$, two symmetric and one antisymmetric SL state at $\chi = 1.6525$ and two symmetric and two antisymmetric SL states for $\chi > 1.6525$.

Now let us consider asymmetric case where $\beta \neq 1$. The effective Hamiltonian is function of two dynamical variables namely, $\beta$ and $\eta$. Therefore the fixed point solutions will obey the equations given by

$$\frac{\partial H_{\text{eff}}}{\partial \eta} = 0 \quad \text{and} \quad \frac{\partial H_{\text{eff}}}{\partial \beta} = 0.$$ \hspace{1cm} (14)

After a little algebra we obtain the desired equation,

$$\frac{1}{\chi} = \frac{\beta(9 - 7\beta^2 - \beta^4 - \beta^6)^2}{2(1 - \beta^2)(3 - \beta^2)^4} = f(\beta).$$ \hspace{1cm} (15)

The function $f(\beta)$ monotonically increases with $\beta$ and it goes to infinity as $\beta$ goes to 1. From this we can immediately see that there always exists one SL state no matter how small $\chi$ may be.

Combining all the possible states we find that there is one SL state for $\chi < 0.7149$, two at $\chi = 0.7149$, three for $0.7149 < \chi < 1.6525$, four at $\chi = 1.6525$ and five for $\chi > 1.6525$. Hence the maximum number of SL states is five. We further note that the critical values for nonlinear strength is lower and the number of SL states are more compared to the results obtained by eq. (1) (with $\sigma=2$) \textsuperscript{[10]}. Thus it is again confirmed that eq. (2) is more effective in the formation of SL states compared to eq. (1).

**IV. FULLY NONLINEAR CHAIN**

We now consider perfectly nonlinear chain \textit{i.e.,} $\chi_n = \chi$. The Hamiltonian for this system is given by eq.(2) with $\chi_n = \chi$. Using the stationarity condition, we can obtain the Hamiltonian in terms of $\phi_n$. In this case it is not possible to find the exact ansatz for
the localized states, but there are a few rational choices. For example, a single site peaked as well as inter-site peaked and dipped solutions are possible. We will consider these cases subsequently. Let us first consider the on-site peaked solution. Without any loss of generality we can assume that the exciton profile is peaked at the central site. Therefore, using the ansatz \( \phi_n = \phi_0 \eta^{|n|} \) and the normalization condition we get the effective Hamiltonian,

\[
H_{\text{eff}} = \frac{4\eta}{1 + \eta^2} + \chi \frac{(1 - \eta^2)^3}{(1 + \eta^2)^3}.
\]  

From the fixed points equation, \( \partial H_{\text{eff}} / \partial \eta = 0 \), we obtain

\[
\frac{1}{\chi} = \frac{3\eta(1 - \eta^2)}{(1 + \eta^2)^2}.
\]  

After analyzing this equation we find that there is a critical value of \( \chi = 1.333 \) below which there is no SL state and above it there are two states. At the critical value of \( \chi \) there is one state.

For the inter-site peaked and dipped solutions we use the ansatz of the dimeric impurity nonlinear impurity. carrying out the calculation involved we obtain the effective Hamiltonian of the reduced dynamical system to be

\[
H_{\text{eff}} = 2\beta \frac{1 - \eta^2}{1 + \beta^2} + 2 sgn(E)\eta - \chi \frac{(1 - \eta^2)^2}{(1 + \beta^2)^2} \left[ \beta^2 + \frac{\eta^2 + \beta^2\eta^2 - 1 - \beta^4}{1 - \eta^4} \right]
\]  

where \( \beta \) is defined earlier. We first consider the case \( \beta = \pm 1 \). Substituting \( \beta = \pm 1 \) into the Hamiltonian and from the fixed points equations we obtain

\[
\frac{1}{\chi \pm} = \frac{\eta(1 - \eta^2)(2 + \eta^2)}{2(\text{sgn}(E) \mp \eta)(1 + \eta^2)^2}.
\]  

Here '+' sign corresponds to the symmetric case and the '-' sign to the antisymmetric case. From eq. (19) it is clear that there will be two critical values of \( \chi \) namely, \( \chi_{cr}^+ = 2.4653 \) and \( \chi_{cr}^- = 5.9178 \). There is no SL state for \( \chi < \chi_{cr}^- \), one SL state for \( \chi = \chi_{cr}^+ \), two SL states for \( \chi_{cr}^- < \chi < \chi_{cr}^+ \), three SL states at \( \chi = \chi_{cr}^- \) and four SL states for \( \chi > \chi_{cr}^- \).

On the other hand for \( \beta \neq 1 \) we find that \( \beta \in [0, 1] \) and \( \eta \in [0, 1] \) satisfy the following equations.
\[-4\beta\eta(1 + \beta^2)(1 + \eta^2)^2 + 2\text{sgn}(E)(1 + \beta^2)^2(1 + \eta^2)^2 + 2\chi\eta[-3 + \beta^2 - \beta^2\eta^4]
\]
\[-\chi[2\eta^2 - 4\beta^2\eta^2 - 2\beta^4 + \eta^4 - 2\beta^2\eta^6] = 0
\]
\[2(1 + \eta^2)(1 + \beta^2)^2 - 4\beta^2(1 + \eta^2)(1 + \beta^2) - \chi[(1 + \beta^2)(2\beta - 2\beta\eta^2\beta^2\eta^2 - 4\beta^3)]
\]
\[+4\chi\beta[\beta^2 - \beta^2\eta^4 + \eta^2 + \beta^2\eta^2 - 1 - \beta^4] = 0 \quad (20)
\]

As it is not possible to decouple the equations, we have obtained numerically the possible values of \(\beta\) and \(\eta\) for various values of \(\chi\). It is found that there is always exists one SL state for any nonzero value of \(\chi\).

Now combining all the possibilities, we obtain the following result for the fully nonlinear chain. There will be only one SL state for \(\chi < 2.4653\), two for \(\chi = 2.4653\), three for \(2.4653 < \chi < 5.9178\), four for \(\chi = 5.9178\) and five for \(\chi > 5.9178\). Hence the maximum number of SL states is five. We further note that SL state appears even if the system is perfect (the translational symmetry is preserved). Therefore, we may call these states to be self-localized states.

V. STABILITY

The stability of the SL states can be understood from a simple graphical analysis. For this purpose, consider the case of single impurity with \(\chi = 1.3\) (for which two SL states appear). The fixed point equation for the single impurity case with \(\chi = 1.3\) is given by

\[G(\eta) = 1 - \frac{\eta(1 - \eta^2)(10 + 2\eta^2)}{(1 + \eta^2)} = 0. \quad (21)
\]

The flow diagram of the dynamical system described by the \(H_{eff}\) given in eq. (6) is constructed in the following manner. We treat \(G(\eta)\) as the velocity and \(\eta\) as the coordinate of the dynamical system. \(G(\eta)\) is plotted as a function of \(\eta\) in fig. (2). 'A' and 'B' are the fixed points corresponding to the SL states. If \(G(\eta) > 0\), the flow of the dynamical variable is in right direction else it is in left. The direction of flow is shown by arrows in different regions. It is clear from the flow diagram 'A' is a stable fixed point whereas 'B' is unstable. Therefore, for the case of single impurity, one state is stable and the other one is unstable.
The energy of the SL states as a function of $\chi$ is plotted in fig. (3). Once again we confine to the single impurity case. It is clear that energy of one state increases and that of the other decreases. (Note that the points 'A' and 'B' of fig.(3) gets mapped to points 'A'' and 'B'' respectively.) Thus we conclude that the states in the upper branch of the energy diagram are stable SL states and those of the lower branch are unstable SL states. In other words, if the energy of SL state increases with the increase of nonlinear strength, the state is stable otherwise, unstable.

VI. CONCLUSION

DNLS given by eq. (2) is used to study the formation of stationary localized states in a one dimensional system with single and a dimeric nonlinear impurity. It is found that the number of SL states are more than the number of impurities in the system. Maximum number of SL states due to single nonlinear impurity is two and that due to dimeric nonlinear impurity is five. It is further found that SL states may appear even in a perfectly nonlinear system. Thus one may call these SL states as self-localized states. It is also interesting to note that eq. (2) is more effective in the formation of SL states compared to eq. (1). The stability of the SL states is discussed and the connection of the stability of a state with its energy variation as a function of nonlinear strength is presented. For a clearer understanding on the effect of nonlinear impurities on the formation of SL states, one needs to consider the presence of a finite nonlinear clusters in a linear host lattice. Investigation in this aspect is in progress and will be reported elsewhere.

VII. ACKNOWLEDGEMENT

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REFERENCES

[1] E. N. Economou, *Green’s Function in Quantum Physics* (Springer-Verlag, Berlin. 1979).

[2] M. I. Molina and G. P. Tsironis, Phys. Rev. B 47 15330 (1993).

[3] M. I. Molina, G. P. Tsironis and D. Hennig, Phys. Rev. E 50 2365 (1994).

[4] M. I. Molina and G. P. Tsironis, Int. Jour. Mod. Phys. B 9 1899 (1995).

[5] Y. Y. Yiu, K. M. Ng and P. M. Hui, Phys. Lett. A 200 325 (1995); Solid State Commun. 95 801 (1995).

[6] P. M. Hui, Y. F. Woo and W. Deng, J. Phys. Condens. Matt. 8 2011 (1996).

[7] A. B. Aceves et al., Phys. Rev. E 53 1172 (1996).

[8] B. Melomed and M. I. Weinstein, Phys. Lett. A 220 91 (1996).

[9] B. C. Gupta and K. Kundu, Phys. Rev B 55 894 (1997).

[10] B. C. Gupta and K. Kundu, Phys. Rev B 55 11033 (1997).

[11] K. Kundu and B. C. Gupta, Euro. Phys. Jour. B 3 (1998).

[12] B. C. Gupta and K. Kundu, Phys. Lett. A 235 176 (1997).

[13] A. Ghosh, B. C. Gupta and K. Kundu, J. Phys. Conden. Matt. 10 2701 (1998).

[14] V. M. Kenkre, G. P. Tsironis and D. K. Campbell, *Nonlinearity in Condensed Matter*, eds. A. R. Bishop et al. (Springer-Verlag, 1987).

[15] V. M. Kenkre and G. P. Tsironis, Phys. Rev. B 35 1473 (1987).
FIGURES

FIG. 1. $f(\eta)$ is plotted as a function of $\eta$. It clearly shows a maximum.

FIG. 2. $G(\eta)$ is plotted as a function of $\eta$. $A$ and $B$ are fixed points.

FIG. 3. Energies of the SL states are plotted as a function of $\chi$. There is no state below $\chi_{cr}$ and two states above it. Energy of one state increases and that of the other decreases. Points $A'$ and $B'$ corresponds to points $A$ and $B$ respectively of Fig. 2.
