Formation of stationary localized states in one-dimensional chain due to a linear impurity and a modified nonlinear impurity is studied. Furthermore, a one-dimensional chain with linear and modified nonlinear site energies at the alternate sites is studied and rich phase diagrams of SL states are obtained for all the systems we considered. The results are compared with those of the linear and nonlinear systems.

I. INTRODUCTION

It is well known that the transport properties of a system is directly related to the formation of stationary localized (SL) states in the system. Localized states appear due to the presence of impurity or disorder (which breaks the translational symmetry) in the system. There has been detailed study on the formation of SL states in various systems in the presence of linear impurities. One the other hand the effect on the formation of localized states due to the presence of nonlinear impurities has been studied recently by the use of the discrete nonlinear Schrödinger equation given as

$$i \frac{dC_n}{dt} = \epsilon_n C_n + V(C_{n+1} + C_{n-1}) + \chi_n |C_n|^\sigma C_n, \quad (1)$$

where $\sigma$ is equal to 2 or arbitrary constant, $C_n$ is the probability amplitude of the particle 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 $|C_n|^\sigma C_n$ arises due to interaction of the exciton with the lattice vibration. If the lattice oscillators are purely harmonic in nature, then $\sigma = 2$. The Eq. (1) has been derived with the assumption that the lattice oscillators are much faster in motion compared to that of the exciton and the lattice oscillators are independent of others. Equation (1) has been used to study the formation of SL states due to a single nonlinear impurity and that due to a dimeric nonlinear impurity in one dimensional chain as well as in a Cayley tree. A perfect nonlinear chain with nonlinear impurity have also been considered to study the SL states and it has been shown that SL states appear even though the translational symmetry of the system is preserved. Very recently the effect of the presence of both the linear and nonlinear impurities in one dimensional chain and in the Cayley tree has been studied and rich phase diagrams of SL states have been obtained. The Eq. (1) may be modified if the lattice oscillators are assumed to be coupled with their nearest neighbors. Thus, under the assumption that the oscillators are coupled to its nearest neighbors and are much faster in motion compared to the motion of the exciton, the discrete nonlinear Schrödinger equation is modified and takes the form:

$$i \frac{dC_n}{dt} = \epsilon_n C_n + V(C_{n+1} + C_{n-1}) + \chi_n |C_n|^\sigma C_n, \quad (2)$$

where $C_n$, $\epsilon_n$, $V$ and $\chi_n$ carries same meaning as for the Eq. (1). The modified discrete nonlinear Schrödinger equation (Eq. (2)) has been derived from the coupled exciton-oscillator system by Kopidakis et al. [20]. We notice that the Eq. (2) contains more nonlinear terms compared to Eq. (1) and, in addition, Eq. (2) is also relevant in condensed matter physics because the nearest neighbor coupling among the lattice oscillators is taken into account in deriving the equation. One interesting property of Eq. (2) is the self-trapping property and this aspect has been studied by Kolosakas et al. [21]. Another interesting property of this equation is that it can produce SL states. In fact the Eq. (2) has been exploited to study the formation of SL states in one dimensional system in the presence of a single nonlinear impurity, and that in the presence of a dimeric nonlinear impurity [22]. The Eq. (2) has also been used to find the SL states in a perfectly nonlinear chain [23]. However the system with both the linear and the modified nonlinear impurities has not been considered yet to study the formation of SL states. Thus we are interested to observe the mixed role of linear and modified nonlinear impurities on the formation of SL states in one dimensional system.

The organization of the paper is as follows. The one dimensional chain with a linear impurity and a modified nonlinear impurity is considered in Sec. I. In Sec. II we consider the one dimensional chain with linear and modified nonlinear impurities at alternate sites of the lattice. Finally In Sec. III we summarize our findings.

II. ONE DIMENSIONAL CHAIN WITH A LINEAR IMPURITY AND A MODIFIED NONLINEAR IMPURITY

Consider a one-dimensional chain consisting of a linear impurity of strength $\epsilon$ placed at the zeroth site and a nonlinear impurity of strength $\chi$ at the first site. The relevant Hamiltonian for such a system can be written as

$$H = \frac{1}{2} \sum_{n=-\infty}^{\infty} (C_n^* C_{n+1} + C_n^* C_{n+1}) + \frac{\epsilon}{2} |C_0|^2$$

\begin{equation}
\frac{8}{\chi^{\pm}} = \frac{\eta(1-\eta^{2})(3\eta^{2}+5)}{\text{sgn}(E) - (\frac{5}{8} \pm 1)\eta} = f_{\pm}(\eta).
\end{equation}

From Eq. (10) it is clear that the states will appear above the band for \( \chi^{+} > 0 \) and below the band for \( \chi^{+} < 0 \). [Note that the band edges are at \( E/V = \pm 2 \).] We will consider positive values of \( \chi^{\pm} \) and, hence, the \( \text{sgn}(E) \) may be taken to be positive. For symmetric states, the value of \( f_{+}(\eta) \) exhibits the extreme values: \( f_{+}(\eta) \to 0 \) as \( \eta \to 0 \) and \( f_{+}(\eta) \to \infty \) as \( \eta \to 1/(\epsilon/2 + 1) \). Thus, \( f_{+}(\eta) \) increases as \( \eta \) increases from \( \eta = 0 \) and diverges at \( \eta = 1/(\epsilon/2 + 1) \), and it becomes negative for \( \eta > 1/(\epsilon/2 + 1) \). This means that there will always be only one solution (symmetric state) for all positive values of \( \epsilon \) and \( \chi \). For antisymmetric states, we found that \( f_{-}(\eta) \to 0 \) as \( \eta \to 0 \) and \( f_{-}(\eta) \to \infty \) as \( \eta \to 1/(\epsilon/2 - 1) \). The divergence of \( f_{-}(\eta) \) is, however, confined between 0 and 1 if and only if \( \epsilon > 4 \). Therefore, for \( \epsilon > 4 \), \( f_{-}(\eta) \) increases as \( \eta \) increases from \( \eta = 0 \), diverges at \( \eta = 1/(\epsilon/2 - 1) \), and finally becomes negative for \( \eta > 1/(\epsilon/2 - 1) \). This implies that there will always be one antisymmetric state for \( \epsilon > 4 \) for any value of \( \chi > 0 \). However, the situation is different for \( \epsilon < 4 \); the value of \( f_{-}(\eta) \) approaches 0 as \( \eta \to 0 \) and \( \eta \to 1 \) and remains positive and finite for \( 0 < \eta < 1 \). This implies that \( f_{-}(\eta) \) has at least one maximum in the range of \( 0 < \eta < 1 \). We confirm by a graphical analysis that there is only one maximum. Therefore, there will be a critical value of \( \chi \) separating two antisymmetric states from the region of no antisymmetric state for \( \epsilon < 4 \). The dashed line in Fig. 1 is such a critical line and is denoted by \( \chi^{a}_{cr} \). Thus, there are three regions in the entire plane of \( \epsilon \) versus \( \chi \), having different number of symmetric and antisymmetric SL states. The region of \( \epsilon > 4 \) has one symmetric and one antisymmetric SL states, while the region of \( \epsilon < 4 \) is divided into two regions by the critical line \( \chi^{a}_{cr} \), below of which has only one symmetric state and above of which has one symmetric state and two antisymmetric states. Therefore, the maximum number of SL states contributed by the symmetric and anti-symmetric solutions is three.

Next, we consider the asymmetric solutions, i.e., for \( \beta \neq \pm 1 \). The effective Hamiltonian in Eq. (8) should be considered as a function of two variables, \( \eta \) and \( \beta \), while \( \epsilon \) and \( \chi \) remain constant for a particular system. The fixed-point solutions corresponding to the SL states can be obtained from the following two extreme conditions

\begin{align}
\frac{\partial H_{\text{eff}}}{\partial \eta} &= 0, \\
\frac{\partial H_{\text{eff}}}{\partial \beta} &= 0.
\end{align}

After a trite algebra, the fixed-point equations reduce to

\begin{align}
\frac{8}{\chi^{\pm}} &= \frac{\eta(1-\eta^{2})(3\eta^{2}+5)}{\text{sgn}(E) - (\frac{5}{8} \pm 1)\eta} = f_{\pm}(\eta).
\end{align}
one modified nonlinear impurity play a role to increase four \[ \text{we thus conclude that one linear impurity and that in one dimensional chain in one dimensional chain with two linear impurities was found to be two [1] and that in one dimensional chain with two modified nonlinear impurities was found to be four [2]}. \]

These coupled equations can not be solved analytically and, accordingly, we analyze them numerically to find the number of asymmetric SL states (number of solutions with \( \eta \in [0, 1] \)).

\[
\begin{align*}
2(1 + \beta^2)(1 + \beta^2 - 2\eta \beta - \epsilon \eta) \\
- \chi \eta (1 - \eta^2)(3\beta^4\eta^2 + 3\beta^4 + 2\beta^2) &= 0
\end{align*}
\]

and

\[
\begin{align*}
2(1 + \beta^2)(1 - \beta^2 - \epsilon \beta) \\
+ \chi \beta (1 - \eta^2)(2\beta^2\eta^2 + 3\beta^2 + 1) &= 0 \quad (12)
\end{align*}
\]

FIG. 1. The phase diagram for SL states in the plane of \( \epsilon \) versus \( \chi \) for a system of a one-dimensional chain with a linear impurity and a modified nonlinear impurity. Different regions are marked with the number of states and the kind of states; the region marked by “1s+2a+2as” means that the region has one symmetric, two antisymmetric and two asymmetric SL states. The small unmarked region has only one symmetric SL state.

It is found that there are three critical lines separating different number of asymmetric SL states in the plane of \( \epsilon \) versus \( \chi \) denoted by the solid curves in Fig. 1. Maximum number of asymmetric SL states obtained is two. Considering all possible states we find that maximum number of SL states is five. The “s”, “a” and “as” (in Fig. 1) stand for symmetric, antisymmetric and asymmetric states, respectively. For example, the region marked as “1s+2a+2as” has one symmetric SL state, two antisymmetric SL states, and two asymmetric SL states. It should be noted that the number of states changes one by one as we go from one region to another in the phase space. As an example, as we cross from the region “1s+1as” to the region “1s+2a+1as”, the number of states increases by two; however, the number of states on the critical line which separates two regions is “1s+1a+1as”, yielding the increment of the number of states one by one. The maximum number of SL states in one dimensional chain with two linear impurities was found to be two [1] and that in one dimensional chain with two modified nonlinear impurities was found to be four [2]. We thus conclude that one linear impurity and one modified nonlinear impurity play a role to increase the maximum number of SL states. The phase diagrams of SL states here is very complicated when compared to the that for one dimensional chain with two modified nonlinear impurities.

Figure 2 shows the variation of energy of the states as a function of \( \chi \) for a fixed value of \( \epsilon = 6 \). We see that three SL states appear at \( \chi = 5 \) as expected from the phase diagram (Fig. 1). The energy of the symmetric state (top solid line in Fig. 2) and that of the antisymmetric state (another solid line in Fig. 2) increases while the energy of the asymmetric state decreases as \( \chi \) increases. At \( \chi \approx 6.06 \) one more asymmetric state appear whose energy increases with the increment of \( \chi \) and finally both the asymmetric states disappear at \( \chi = 6.55 \). Thus we find that the symmetric state and the antisymmetric state are strongly localized compared to the asymmetric states in the parameter regime considered in Fig. 2. Through stability analysis [22] it can be shown that the state whose energy decreases with the increment of \( \chi \) is unstable.

FIG. 2. Variation of energy as a function of \( \chi \) is shown for \( \epsilon = 6 \).

### III. LINEAR AND MODIFIED NONLINEAR SITE ENERGIES AT ALTERNATE SITES

In this section, we consider a one-dimensional chain with alternate site energies; the even sites have a linear energy \( \epsilon \) and the odd sites have a modified nonlinear energy \( \chi \)\(|C_{n+1}|^2 + |C_{n-1}|^2 + 2|C_n|^2\). Such a system can be described by the Hamiltonian given as

\[
H = \frac{1}{2} \sum_{n=-\infty}^{\infty} (C_n^* C_{n+1} + C_n^* C_{n-1}) + \frac{\epsilon}{2} \sum_{n=-\infty}^{\infty} |C_{2n}|^2 + \chi \sum_{n=-\infty}^{\infty} (|C_{2n+2}|^2 + |C_{2n-2}|^2 + 2|C_{2n+1}|^2)|C_{2n+1}|^2. \quad (13)
\]

For \( \chi = 0 \), the system reduces to a periodically modulated linear system. The translational symmetry of the system is preserved for both \( \chi = 0 \) and \( \chi \neq 0 \). Using \( C_n = \phi_n \exp(-iEt) \), we obtain the Hamiltonian in terms of \( \phi_n \). It is, however, not possible to find the exact ansatz for the localized states in this system, although a
certain rational ansatz can be considered. For example, the on-site peaked solution, inter-site peaked or inter-site dipped solutions are possible. We will consider each of these in the subsequent subsections.

![Diagram](image)

FIG. 3. The phase diagram of SL states in the $\epsilon$ versus $\chi$ plane for the system of a one dimensional chain with linear and modified nonlinear site energies at alternate sites. The number ‘2’ added in every region indicates that there are two on-site peaked states apart from the symmetric, antisymmetric and asymmetric states; one of them is peaked at the linear site and another one is peaked at the nonlinear site. For example, the region marked by ‘1s+2a+1as+2’ has one symmetric state, two antisymmetric states, one symmetric state and two on-site peaked states (one peaked at the linear site and another one peaked at the nonlinear site).

**A. On-site peaked solution**

Since the system has linear and nonlinear sites at regular intervals, the solution may have a peak either at the linear site or at the nonlinear site. We first consider the solution peaked at the linear site, i.e. the solution is peaked at the central site of the system. We therefore consider the ansatz $\phi_n = \phi_0 \eta^n$. Using this and the normalization condition, we obtain the effective Hamiltonian as

$$H_{\text{eff}} = \frac{2\eta}{1 + \eta^2} + \frac{\epsilon}{2} \frac{(1 + \eta^2)}{(1 + \eta^2)^2} + \frac{\chi}{2} \frac{\eta^2(1 - \eta^2)}{(1 + \eta^2)(1 + \eta^2)}. \quad (14)$$

The fixed-point equation, $\partial H_{\text{eff}} / \partial \eta = 0$, reduces to

$$2(1 - \eta^8)(1 - \eta^4) - 2\eta(1 - \eta^2)(1 + \eta^4)^2$$

$$+ \chi \eta(1 - \eta^2)^2(1 - 2\eta^2)(1 + \eta^4)$$

$$- \eta^2(1 - \eta^4)(1 + 2\eta^2 + 3\eta^4) = 0. \quad (15)$$

Solving Eq. (15), we found that there is always one SL state peaked at the linear site for any value of $\epsilon$ and $\chi$. The localized solution peaked at the nonlinear site may be obtained considering that each site is shifted by one lattice site along either positive or negative direction, and the resulting fixed-point equation is given as

$$2 \left(1 + \eta^2 \right)(1 - \eta^4)^2(1 - \eta^8)^2 + 2\eta(1 - \eta^4)(1 - \eta^8)^2$$

$$+ \chi \eta \left(1 + \eta^2 \right)^2(1 - \eta^8)^2(1 - 3\eta^2) + 8\eta^6(1 - \eta^4)^2$$

$$- \chi \eta \left(4(1 - \eta^4)(1 - \eta^8)^2 + 3\eta^2(1 - \eta^2)(1 - \eta^8)^2 \right) = 0. \quad (16)$$

It is found from the analysis of Eq. (16) that only one SL state peaked at the nonlinear site appears irrespective of the values of $\chi$ and $\epsilon$.

**B. inter-site peaked and dipped solutions**

For the inter-site peaked and dipped solutions we use the dimeric ansatz in Eq. (5). After short calculations, we obtain the effective Hamiltonian for the reduced dynamical system as

$$H_{\text{eff}} = \text{sgn}(E)\eta + \frac{\beta(1 - \eta^2)}{1 + \beta^2} + \frac{\epsilon}{2} \frac{(1 + \beta^2)\eta^2}{(1 + \eta^2)(1 + \eta^2)}$$

$$+ \frac{\chi(1 - \eta^2)^2}{4(1 + \beta^2)} \left[ \frac{\eta^2(1 + \beta^2)^2}{(1 - \eta^8) + \beta^2} \right]$$

$$+ \frac{\chi(1 - \eta^2)^2}{4(1 + \beta^2)\eta^2} \left[ \frac{\eta^6(1 + \beta^4)}{(1 - \eta^8)} + \frac{(\beta^4 + \eta^4)}{(1 - \eta^8)} \right] \quad (17)$$

with $\beta$ and $\eta$ as defined earlier. We first consider the symmetric and antisymmetric states, i.e., $\beta = \pm 1$. The fixed-point equation yields

$$\frac{4}{\chi^{\pm}} = \frac{\eta \left[(1 + \eta^2)(1 + 2\eta^2 - \eta^4) - \eta^4 \right]}{(1 + \eta)(1 + \eta^2)^2} = f^{\pm}(\eta), \quad (18)$$

where “$+$” refers to the symmetric states and “$-$” to the antisymmetric states. It should be noted that $\epsilon$ has no role in the formation of symmetric and antisymmetric SL states in the system. From Eq. (18) it is clear that only one symmetric state appears for any finite value of $\chi$. However, for antisymmetric states, the situation is different. The value of $f^{\pm}(\eta)$ in Eq. (18) initially increases as $\eta$ increases and finally decreases as $\eta$ approaches to 1, leaving a maximum at $\eta \in [0, 1]$. Thus, there are two critical values of $\chi$ such that there is no anti-symmetric SL state for $\chi < 9.07$, two anti-symmetric SL states for $9.07 < \chi < 10.66$ and one anti-symmetric SL state for $\chi \geq 10.66$, shown as the two vertical lines in Fig. 3.

We next consider the asymmetric states of $\beta \neq 1$. In this case $\epsilon$ plays its role, unlike the case of symmetric and antisymmetric states. The fixed-point equations are given as

$$\left[(1 + \eta^2)^2(1 + \beta^2)(1 + \beta^2 - 2\beta\eta) - \epsilon\eta(1 - \beta^4)\right]$$

$$+ \chi\eta(1 - \eta^2)^2(1 - \eta^8)$$

$$\left[\frac{1}{2}(1 + \beta^4)(1 + 3\eta^2) - \beta^2(1 + \eta^2)(1 + \eta^4) + \eta^2 \right]$$

$$+ \chi\eta^3(1 - \eta^4)(1 - \eta^8)(1 + \beta^4)$$

$$\left[2\eta^6 - (1 + \eta^2)(1 + \eta^4) \right]$$

$$- \chi\eta(1 - \eta^4)^2(\beta^4 + \eta^4)(1 + \eta^2 + \eta^4 - \eta^6) = 0$$

and

$$\left[(1 + \eta^2)^2(1 - \eta^8)^2 + 2\eta(1 - \eta^4)(1 - \eta^8)^2$$

$$+ \chi\eta \left(1 + \eta^2 \right)^2(1 - \eta^8)^2(1 - 3\eta^2) + 8\eta^6(1 - \eta^4)^2$$

$$- \chi\eta \left(4(1 - \eta^4)(1 - \eta^8)^2 + 3\eta^2(1 - \eta^2)(1 - \eta^8)^2 \right) = 0. \quad (16)$$
Solving Eqs. (19) and (20) we obtain two critical curves (solid curves in Fig. 3) separating the $\chi - \epsilon$ plane into various regions with various number of asymmetric SL states as shown in Fig. 3. Symmetric states are denoted by ‘s’, antisymmetric states are denoted by ‘as’ and asymmetric states are denoted by ‘as’. The region marked by ‘1s+2a+1as+2’ contains one symmetric SL state, two antisymmetric SL states, one asymmetric SL state, one SL state peaked on the nonlinear site and one SL state peaked at the linear site. The maximum number of states obtained in this case is 6 which is the same as for the chain with modified nonlinear impurities of different strengths at alternate sites. Thus in this case the linear impurity plays the same role as that of nonlinear impurity to obtain the maximum number of SL states. No SL state is obtained for $\chi = 0$. This is expected because the system with $\chi = 0$ reduces to a periodically modulated linear system which again may be renormalized to a perfect linear system.

IV. SUMMARY

Formation of stationary localized states in one dimensional chain due to the presence of a linear impurity and a modified nonlinear impurity is studied. Maximum number of SL states in this case is found to be five which is larger than that obtained for a one dimensional chain with two modified nonlinear impurities. Thus one may conclude that the presence of both linear and nonlinear impurities plays a role to increase the maximum number of SL states. The variation of energy of SL states as a function of the nonlinear strength for a fixed value of linear impurity strength is presented. It is found that the symmetric and antisymmetric states are strongly localized when compared with the asymmetric states.

Furthermore, a one dimensional chain with linear and modified nonlinear energies at alternate sites is considered. Here the maximum number of SL states is found to be six. The linear energy strength at alternate sites in the chain does not play any role to produce the symmetric and antisymmetric SL states and the system does not produce any SL state for $\chi = 0$ which is expected. However, surprisingly, the linear energy strength plays a role to produce the asymmetric SL states. Rich phase diagrams of SL states for both the systems considered here are presented.

\[
(1 - \eta^8)(1 - \eta^4)(1 - \beta^4)
\]
\[-\epsilon \beta (1 - \eta^8)(1 + \beta^2)(1 - \eta^2)
\]
\[+ \chi \beta (1 - \eta^2)(1 - \eta^4)(1 + \beta^2)
\]
\[
\left[ (1 - \eta^8) + \beta^2 (1 + \eta^2 + \eta^6) \right]
\]
\[-\chi \beta (1 - \eta^2)(1 - \eta^4)(\eta^2 + \beta^4)(1 + \eta^4)
\]
\[+ \beta^4 (1 - \eta^8) + \beta^4 + \eta^8 \right] = 0 \tag{20}
\]

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