Multi-polaron solutions, nonlocal effects and internal modes in a nonlinear chain

N. Bondarenko,¹ O. Eriksson,¹,² N. V. Skorodumova,¹,³ and M. Pereiro¹

¹Division of Materials theory, Department of Physics and Astronomy, Uppsala University, Box 516, 75121 Uppsala, Sweden
²School of Science and Technology, Örebro University, SE-70182 Örebro, Sweden
³Multiscale Materials Modelling, Department of Materials Science and Engineering, Royal Institute of Technology, SE-10044 Stockholm, Sweden

Multipolaron solutions were studied in the framework of the Holstein one-dimensional molecular crystal model. The study was performed in the continuous limit where the crystal model maps into the nonlinear Schrödinger equation for which a new periodic dnooidal solution was found for the multipolaron system. In addition, the stability of the multi-polaron solutions was examined, and it was found that cnoidal and dnooidal solutions stabilize in different ranges of the parameter space. Moreover, the model was studied under the influence of nonlocal effects and the polaronic dynamics was described in terms of internal solitonic modes.

I. INTRODUCTION

During the last decades, it has widely been recognized in many areas of physics [1–4] that nonlinearity can turn into a fundamentally new phenomena, which cannot be constructed via perturbation theory, and new mathematical tools are required. The polaron theory which describes a carrier interacting with the lattice vibrational degrees of freedom is undoubtedly a good illustration of this principle [5]. This fascinating object reveals fundamental importance for both physics and mathematics, indeed fortifying the basal relationship of the two disciplines [6, 7].

In earlier works, it has been shown that the tight-binding polaron Hamiltonian can be mapped into a Nonlinear Schrödinger Equation (NLSE) [8, 9] where a solitonic solution of NLSE corresponds to a single polaron. Despite the apparent simplicity, the result had paramount importance for polaron theory mirroring its relationship with other fundamental nonlinear models described, for example, by the Gross-Pitaevskii [10, 11], Klein-Gordon [12, 13] or Ginzburg-Landau [14] equations. Later the solution tree of the polaronic NSLE was expanded to Jacobi elliptic functions [15]. It was shown that in addition to the robust and stable solitonic solution, periodic cnoidal waves can also stabilize. Numerical simulations have justified the obtained analytical results [16] and reported on the chaotic and stochastic behavior of the 1D polaronic system [16, 17]. The majority of these seminal studies on 1D single polaron motion consider a local character of the electron-phonon effects while non-local interaction demands a better understanding [18, 19]. Thus, in the case of strongly nonlocal nonlinearity, several new states can emerge as, for example, chaotics which exhibit both chaotic and soliton-like properties [20]. Moreover, external perturbations induced by non-local effects also destroy the complete integrability of the NLSE and consequently, the inelastic collision among interacting solitons emerges. In Klein-Gordon type models, the effect is attributed to the excitation of internal modes [21] which, within the molecular model, can be considered as phonons coupled to the localized charge state [22]. Thus, the trends obtained by the polaronic model formulated in the NLSE framework can describe successfully the mesoscopic phenomena recently observed in experiments like, for example, charge density wave stabilization in (high-$T_c$) superconductors [23] and localized charge dissipation due to internal mode excitation [24].

The paper is organized as follows. In Section II we present model describing 1D electron-lattice chain and formalism applied to map the corresponding Hamiltonian to NLSE. Next, in Section III we present an analytical analysis of the solution hierarchy of the continuous NLSE in the case of the 1D polaron model. In Section IV we report on modulation instability of periodic solutions. Numerical modeling of the system behavior with a finite, extended nonlocal term is studied in Section V. Moreover, in Appendices we discuss some mathematical and numerical aspects highlighting the results presented in the paper. In Appendix A, we analyze the families of solutions obtained using the G'/G expansion method [25] while in Appendix B, we performed simulations with different set of parameters for the extended NLSE. Possible excitation of internal modes in the extended NLSE is discussed in Appendix C. The work concludes in Section VI.

II. MODEL

We start from the electron-lattice Hamiltonian in the frame of the Holstein molecular-crystal model [9]:

\[
H = - j \sum_n a_n^\dagger (a_{n+1} + a_{n-1}) - \sum_n \frac{1}{2} M \omega_n^2 x_n^2 - g \sum_n x_n a_n^\dagger a_n + \sum_n W_n a_n^\dagger a_n,
\]

where $a_n^\dagger$ and $a_n$ denote electronic creation and annihilation operators of the n-th site, respectively. The first
term stands for electrons hopping between lattice sites, in a tight-binding description, with the nearest-neighbor overlap integral \( j \). The second term describes the lattice part of the Hamiltonian in the adiabatic limit. In this description each nucleus with mass \( M \), harmonically oscillate around the stationary center of mass with Einstein frequency \( \omega_0 \) and deviation \( x_n \), estimated with respect to the equilibrium interatomic separation. The third term describes the electron-lattice interaction with the characteristic coupling constant \( g \). Finally, the nonlocal term \( W_n(x_1,\ldots,x_n) \) is assumed to be taken in the form of the Pöschl-Teller potential [26].

Following Holstein's seminal paper [9], the full electronic wave function is expressed as \( |\Psi_e\rangle = \sum a_n |n\rangle \) and hence the electronic amplitude is defined as \( a_n = \langle n|\Psi_e\rangle \). Reformulated in the electronic amplitudes and minimised with respect to the ionic displacements near its equilibrium point for a nonlocal model as described by Eq. (1), the vibration coordinates are \( X_n = \Upsilon_n|a_n|^2 \) with \( \Upsilon_n = \frac{g_{\text{eff}}}{M\omega_0^2} \) [9, 15, 16]. In the continuum limit, the Schrödinger-type eigenvalue problem, in Eq. (1), can be mapped into a NLSE-type of equation:

\[
\frac{\partial^2 a_n}{\partial t^2} + g\Upsilon_n |a_n|^2 a_n - (\varepsilon + W_n)a_n = 0, \tag{2}
\]

where the energy of the localized electron \( \varepsilon = -E + \frac{1}{2} \sum_n M\omega_0^2 X_n^2 - 2j \) is defined in terms of the minimized total energy \( E \) of the 1D chain. Notice that \( a_n \) represents the continuous extension of the electronic amplitude at \( n \). Index \( n \) in this case indicates that \( a_n \) is a continuous variable and a function of \( n \).

### III. PERIODIC SOLUTIONS

In the absence of nonlocality \( (W_n = 0) \), Eq. (2) has several hierarchies of solutions like the self-trapped solitonic solution in the case of electronic states decaying at infinity \( (a_n \to 0 \text{ as } n \to \infty) \) [9, 15], non-decaying Bloch-like solutions [9]. Among the periodic solutions, it is worthy to emphasize the solutions given by Jacobi elliptic functions as the already reported cnoidal solutions [15] and also, a previously not discussed, dnoidal solution (superscripts \( (cn) \) and \( (dn) \), hereafter, denote quantities describing cnoidal and dnoidal solutions, respectively):

\[
a_n^{(cn)} = \frac{m^2}{\sigma} \zeta^{(cn)}(\xi, m); \quad \zeta^{(cn)} = \frac{(\xi)^\frac{1}{2}}{\sqrt{2m - 1}};
\]
\[
a_n^{(dn)} = \frac{\zeta^{(dn)}(\xi, m)}{\sigma^2} d\xi; \quad \zeta^{(dn)} = \frac{(\xi)^\frac{1}{2}}{\sqrt{(2 - m)^2}}.
\tag{3}
\]

where \( \sigma = \frac{g_{\text{eff}}}{4M\omega_0^2} \). The parameter \( m \in [0,1] \) is equal to the square of the modulus of the elliptic function. By using the normalisation condition \( \int |a_n|^2 dn = 1 \) and introducing \( \tilde{\varepsilon} = \frac{\sigma^2 K}{8M\omega_0^2} \), where \( \eta \) stands for half of the chain length, the energy of the localised electron for the two solutions results in (Fig. 1a,b):

\[
\varepsilon^{(cn)} = \frac{2m - 1}{E - m\varepsilon}; \quad \varepsilon^{(dn)} = \frac{2}{E - \varepsilon}.
\tag{4}
\]

Here \( E \) and \( K \) represent the elliptic integral of the first and second kind, respectively while \( m' = 1 - m \). The solutions have limits where the main function collapses either into a harmonic function \( (\text{Jacobi } \text{cn}(u,0)) \) or constant \( (\text{Jacobi } \text{dn}(u,0)) \). Moreover, both solutions converge to the multi-noninteracting soliton solution at \( m \to 1 \) [15] among which the charge carrier has been spread over.

In Appendix A we also derive other periodic and solitonic solutions of NLSE equation using the G'/G expansion [25]. In the next section, we continue studying cnoidal and dnoidal solutions (Eq. (3)), which we consider of primary interest for the presented physical model.

### IV. ON MODULATION INSTABILITY OF THE PERIODIC SOLUTIONS

In order to further clarify the behavior of the multipo- laronic system we suggest the following stability analysis of the cnoidal and the new, dnoidal solution. The starting point is the local, time-dependent analogue of Eq. (2):

\[
\frac{i\hbar}{\tau} \frac{\partial a_n}{\partial \tau} + j \frac{\partial^2 a_n}{\partial n^2} + g\Upsilon |a_n|^2 a_n - W a_n = 0. \tag{5}
\]

The parameter \( \Upsilon = \frac{g_{\text{eff}}}{m\omega_0^2} \) and the last term on the left hand side of Eq. (5) stands for an external homogeneous potential. According to the Lyapunov’s Direct Method the asymptotic stability of a dynamical system can be examined by applying a weak perturbation to the linearized system near its equilibrium. According to the method, we consider the perturbed solution of Eq. (5) in the form of a traveling wave function

\[
A(f(\xi) + \phi_1(\xi, \tau) + i\phi_2(\xi, \tau))e^{i(A^2-k^2)\tau+ikx}.
\tag{6}
\]

In the ansatz represented by Eq. (6), \( A \) is the wave amplitude, \( 2k \) has the meaning of the wave velocity, \( \xi = A(x - 2k\tau) \) and \( \tau = \frac{\tau}{\hbar} \) are new spatial and time variables, respectively. Finally \( f(\xi) \) stands for an unperturbed, periodic kernel which solves the stationary, local (if \( W_n = \text{const} \)) NLSE given by Eq. (2). Substituting the ansatz into Eq. (5), leads us to the following system
of equations
\[ f'''(\xi) + f'(\xi) - \omega f(\xi) = 0; \]
\[ \frac{\partial \phi_1(\xi, \tau)}{\partial \tau} = A^2 (\omega - f^2(\xi) - \frac{\partial^2}{\partial \xi^2}) \phi_2(\xi, \tau) = A^2 \hat{\mathcal{O}}_1 \phi_2(\xi, \tau); \]
\[ i \frac{\partial \phi_2(\xi, \tau)}{\partial \tau} = -i A^2 (\omega - 3f^2(\xi) - \frac{\partial^2}{\partial \xi^2}) \phi_1(\xi, \tau) = -i A^2 \hat{\mathcal{O}}_2 \phi_1(\xi, \tau). \]

Here we find it convenient to introduce the dimensionless parameter \( \omega = 1 + \frac{q \nu}{\beta^2} \). Moreover, \( \hat{\mathcal{O}}_1 \) and \( \hat{\mathcal{O}}_2 \) are the operators acting in the real and complex space, respectively.

After some simple algebra from Eq. (7), we obtain the following relation:
\[ \frac{\partial^2 \phi_1(\xi, \tau)}{\partial \tau^2} = -A^4 \hat{\mathcal{O}}_1 \hat{\mathcal{O}}_2 \phi_1(\xi, \tau). \]

Next, the perturbation term we suggest to be factorized by time as
\[ \phi_1(\xi, \tau) = \phi_1(\xi)e^{A^2 \theta \tau}, \]
where \( \theta \) denotes the instability increment of the system. The stationary part of the perturbation we considered in the form of the Bloch waves \( \phi_{1,2}(\xi) = \sum q f(\xi)e^{iq\xi} \).

In its turn, the periodic kernel in the ansatz has been taken in the form \( \hat{f}(\xi) = \sum_n C_n e^{i(n+q)\xi} \), where \( C_n \) are the coefficients of the Fourier expansion. For further analysis we have also introduced parameter \( Q = q/q_0 \), where \( q \) and \( q_0 \) are main numbers of Bloch envelope and periodic kernel \( \hat{f}(\xi) \), respectively.

To calculate the instability increment introduced in Eq. (9) we follow a formalism previously suggested in plasma physics in order to study modulation instability of the periodic waves [27]. First, we multiply Eq. (8) by \( e^{-i q_m \xi} \) and then integrated the obtained relation over \( l \), the period of function \( \hat{f}(\xi) \). Performing this procedure we have obtained following relation:
\[ \frac{1}{l} \sum_n C_n \int_0^l e^{-i q_m \xi} \hat{\mathcal{O}}_1 \hat{\mathcal{O}}_2 e^{i q_n \xi} d\xi = \sum_n \Theta_m n C_n = -\theta^2 C_m. \]

Taking into account Eq. (9) we can see that the stability analysis can be performed solving eigenvalue problem provided in Eq. (10). The condition of the stability in terms of the \( \Theta_{mn} \) matrix eigenvalues is satisfied when \( -\theta^2 \in \mathbb{R}_+ \). In case of \( -\theta^2 \in \mathbb{R}^- \) or \( -\theta^2 \in \mathbb{C} \) the system instability exponentially diverges with time.

Replacing the operators in Eq. (10) by using Eq. (7) and substituting the periodic kernels in form of the Jacobi elliptic functions (see Eq. (3)), we obtain the explicit form of the \( \Theta_{mn} \). For the cnoidal solution it takes the following form (integrals are normalised with respect to \( l \)):
\[ \Theta^{(cn)}_{mn} = \omega^2 \{(1 + \frac{\pi (Q + n)}{2K(2m - 1)\tau})^2 \delta_{mn} + 3 \frac{2}{2m - 1} \int_0^1 \text{cn}[4K\xi, m]^4 \cos[2\pi(n - m)\xi] d\xi - \frac{2m}{2m - 1} \int_0^1 (4 + 3 \frac{\pi (Q + m)}{2K(2m - 1)\tau})^2 + (\frac{\pi (Q + n)}{2K(2m - 1)\tau})^2 \text{cn}[4K\xi, m]^2 \cos[2\pi(n - m)\xi] d\xi}, \]

and for the dnoidal:
\[ \Theta^{(dn)}_{mn} = \omega^2 \{(1 + \frac{\pi (Q + n)}{K(2 - m)\tau})^2 \delta_{mn} + 3 \frac{2}{2m - 1} \int_0^1 \text{dn}[2K\xi, m]^4 \cos[2\pi(n - m)\xi] d\xi - \frac{2}{2m - 1} \int_0^1 (4 + 3 \frac{\pi (Q + m)}{K(2 - m)\tau})^2 + (\frac{\pi (Q + n)}{K(2 - m)\tau})^2 \text{dn}[2K\xi, m]^2 \cos[2\pi(n - m)\xi] d\xi}. \]

It can be seen that the the eigenvalues \( -\theta^2 \) of infinite dimensional matrix \( \Theta_{mn} \) form a band structure with respect to \( m \) and \( Q \) parameters. In practice, to perform a numerical diagonalisation of Eqs. (11-12), a square matrix with a finite size has been considered. In order to examine matrix size effects we have diagonalised 7x7,
parameters and can be considered as an universal solution. The next notable region is \( \mathbf{m} \gtrsim 0.75 \) where the real part of \(-\theta^2(\text{dn})\) (Fig. 1d) becomes positive and the dnoidal waves stabilize. Further, at \( \mathbf{m} \to 1 \) the instability of the cnoidal solution also monotonically reduces and hence the periodic solutions converge to the robust stable soliton solution.

V. EXTENDED MODEL WITH NON-ZERO NONLOCALITY

Now, gradually increasing the complexity of the problem we consider a nonlocal form for the overlap integral and an inhomogeneous nonlocality. Using a single-site diatomic potential taken in the form of the Pöschl-Teller potential [26], the nonlocal term and hopping integral can be recast in the form

\[
W_n = -\sum_{p\neq n} \gamma_n^2 V_p \int_{-\eta}^\eta \text{sech}^4 \left( \frac{x - x_n}{\beta a} \right) \text{sech}^2 \left( \frac{x - x_p}{\beta a} \right) dx;
\]

\[
j_{nm} = -\gamma_n^2 V_n \int_{-\eta}^\eta \text{sech}^2 \left( \frac{x + x_n}{\beta a} \right) \cosh^4 \left( \frac{x + x_p}{\beta a} \right) dx,
\]

where \( V_p \) is the height of the potential at site \( p \), \( a \) is the lattice constant and \( \beta \) is the parameter accounting for the number of neighbouring shells over which the potential is spread over. Moreover, \( \gamma_n \) represents the maximum of the single-site electron wave function. Since the nonlocal term represents a small perturbation with respect to the rest of the energy terms described in the hamiltonian of Eq. (1), it is reasonable to define an unique hopping constant for the whole system as \( j = (\sum_\delta j_{n\delta} \theta^2) \) where \( j_{n\delta} \) stands for the hopping to the arbitrary \( \delta \)-th nearest neighbour with respect to n-site and \((...)\) denotes the average value over n-sites. Consequently, the extended time-dependent continuous nonlocal NLSE corresponding to Eq. (2) reads as

\[
\imath \hbar \frac{\partial a_n}{\partial t} + j \frac{\partial^2 a_n}{\partial n^2} + g T_n |a_n|^2 a_n - (\varepsilon + W_n)a_n = 0. \tag{14}
\]

The standard NLSE belongs to the class of completely integrable differential equations, for which an infinity of invariants or conservations laws can be obtained by using, for example, the inverse scattering method [29] or Lax Theory [30]. Full integrability is a necessary condition to apply any of these methods to Eq. (14). A simple way to determine the integrability of Eq. (14) is based on the Painlevé test [31]. Passing the Painlevé test is necessary, but not sufficient condition for having the Painlevé property which is defined as the absence of movable critical points or singularities of the solutions of any ordinary differential equation (ODE). It was conjectured that any ODE satisfying the Painlevé property is also fully integrable [32]. A necessary condition for Eq. (14) to pass
the Painlevé test is that $j(g \Upsilon_n)^2 = \mathcal{A}(t)$, where $\mathcal{A}(t)$ is a time-dependent function \cite{33}. Equation (14) does not meet this requirement because $\Upsilon_n$ is not only a time-dependent but also an spatial-dependent function via $n$ and consequently, Eq. (14) is nonintegrable. When the nonintegrable perturbation $W_n$ is small, the equation becomes nearly integrable and still can be solved analytically in a perturbative fashion \cite{32}. In general, if the nonlocal term is big enough and perturbation theory is not applicable, a numerical method can be used instead to get the solution of Eq. (14) and this is the choice adopted here.

After numerically solving the extended time-dependent continuous NLSE for a 1D chain with periodic boundary conditions, we obtain the time-evolution of two localised Gaussian perturbations initially located at positions $n = 5$ and $n = -5$ (Fig. 2). Thus, the initial condition for solutions to Eq. (14) read as

$$a_n(t=0) = \frac{1}{2} \left( e^{-(n-5)^2} + e^{-(n+5)^2} \right). \quad (15)$$

With the aim to emphasize the influence of the nonlocal term, in Fig. 2a)-(c) we plot polaronic and unfocused solutions for a moderately weak nonlocal term, respectively while in Fig. 2b)-(d) we plot the same solutions but with $W_n = 0$. We denote hereafter solutions with $W_n = 0$ as standard solutions. Notice that we used the same material parameters for calculating both kind of solutions of Eq. (14) with the only exception that for the unfocused solution, the nonlinear term was kept bigger ($\sqrt{M\omega_0} = 3.87 \cdot 10^{-2} eV^{0.5} Å^{-1}$) than the one for the solitonic solution ($\sqrt{M\omega_0} = 1.29 \cdot 10^{-2} eV^{0.5} Å^{-1}$). It is also worthwhile to mention that localized electron energy $\varepsilon$ had the same numerical value, for the solution with and without nonlocal term, as indicated in Table I.

Mathematically this approximation is valid when nonlocal perturbations $W_n$ are slowly changing in space, so that, the derivative of $W'_n$ is almost a constant. As shown in Fig. 2, the consequence of the nonlocal term is an asymmetry of the solution with respect to the spatial dimension. Moreover, the nonlocal solution clearly deviates from the standard solution as time evolves. For example, when nonlocal effects are included, the collision of solitons ceases at about 50 fs in Fig. 2a) while it takes longer time for the standard solution, around 300 fs. Thus, this demonstrates, that even for moderately small values of the nonlocal term, its effects are considerable, particularly for longer periods of time. This is also clearly shown in Fig. 2c)-(d) where in the time range from 700 to 800 fs, the nonlocal solution gets more asymmetric than the standard one. The asymmetry is corroborated through the $\Upsilon_n$ term in Eq. (14) which has a functional dependence on $W'_n$, an odd function with respect to the spatial coordinate. After performing simulations with different sets of parameters, as reported in Appendix B, we have noticed that the time evolution and consequently the asymmetry of the nonlocal solution depends strongly on minute variations of $\gamma_n$ and $V_p$ parameters. Moreover, we find that polaron-polaron interaction depends on the strength of the Pöschl-Teller potential and the distance between the polarons.

Further, analyzing the time evolution of both excitations in Fig. 2a)-(b) one can see that both polarons oscillate with respect to the common center of mass and after some time repel each other. In our case, in the region of atomic positions with $|n| > 5$ (see Fig. 2a)-(b)), the excitations have an attractive interaction while in the inner region ($|n| < 5$) the interaction between the excita-
tions becomes repulsive. Thus, the excitations turn into a bipolaron-like oscillating bound pair. The behaviour is typical for the biquadratic trinomial type of potential provided by the first integral of NLS equation. In the case of the extended time-dependent continuous NLS equation, the time evolution of the system is more complex. In this case, we suggest that the system admits internal modes (for more details see Appendix C). If the velocity or the energy of the polaronic excitation is large enough, it may happen that the energy during the collision is transferred to the internal mode. This situation gives rise to an inelastic collision, and consequently, the two excitations escape from their attractive potential well. Moreover, nonlocality interpreted as an external perturbation, shortens the lifetime of the bound state as shown in Fig. 2a)-b). Since the internal modes refer to a localised solution of Eq. (14), the energy in the polaron-polaron collision is preserved. Thus, if the collision excites the internal mode, a subsequent collision can de-excite it. The NLS equation is time-reversal invariant [34]. Consequently, if both excitations come to a second collision in which the phases of the internal modes of both polarons are coherent to the phases in a previous collision, then the second collision will be the time reversal of the first collision. The second collision will cancel out the excitation of the internal modes so that both polarons will recover enough kinetic energy to escape from the attractive potential and break apart the bound state.

VI. CONCLUSION

In summary, we have studied multi-polaron solutions in the framework of the 1D Holstein model. We found that the periodic solutions can stabilize in the certain range of the parameters. We emphasize the importance of the universal, dnoical solution, which previously has not been discussed in the context of the Holstein model. Moreover, the Holstein molecular crystal model in the continual limit was extended and studied under the influence of nonlocal effects. Particularly, we have observed that nonlocal effects influence polaron-polaron collisions by inducing an inelastic scattering via the excitation of internal modes. We show that nonlocality forces the bipolaron dynamics to develop the spatial asymmetry and delocalizes bound polaronic states earlier in time than the standard solution. This later result should also be considered in theories dealing with bipolaronic superconductivity.

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APPENDIX A

The $G'/G$-expansion method was first introduced in Ref. [25] and it is extensively used to search for several exact solutions of time-dependent nonlinear equations [35, 36]. The method is based in linearising the solution in the travelling wave ansatz. Mathematically, the current method maps the nonlinear equation into a second order differential equation with constant coefficients and the problem is reduced to a simple algebraic computation. Further details about the method can be found in Ref. [25].

Let us then start by considering the one-dimensional extended time-dependent nonlinear Schrödinger equation (NLS) with constant coefficients

$$i \frac{\partial \phi(x,t)}{\partial t} + R \frac{\partial^2 \phi(x,t)}{\partial x^2} + S |\phi(x,t)|^2 \phi(x,t) - T \phi(x,t) = 0$$

where $R, S$ and $T$ are real constant coefficients and $\phi(x,t)$ represents the electron wave function at the position $x$ and time $t$. As the NLS equation is complex, we look for a solution factorised as:

$$\phi(x,t) = A U(x,t) e^{i((A^2-k^2)t+Kx)}$$

where $A$ is the amplitude of the wave function, $k$ represents the wave vector and $U(x,t)$ is a complex function. Now inserting Eq. (17) in Eq. (16), taking the appropriate derivatives of $\phi$ and after some algebra, Eq. (16) can be recast in the form:

$$i \frac{\partial U(x,t)}{\partial t} + R \left( \frac{\partial^2 U(x,t)}{\partial x^2} + 2 \frac{\partial U(x,t)}{\partial x} ik \right) + S U^3(x,t) + (k^2 - T - A^2 - Rk^2) U(x,t) = 0$$

Now, by using the travelling wave ansatz, we define $\xi = \frac{x}{R} - 2kt$ so that $U(x,t) = U(\xi)$. Consequently, Eq. (17) can be written in terms of the new variable $\xi$ as:

$$\frac{1}{R} \frac{d^2 U(\xi)}{d\xi^2} + S U^3(\xi) + (k^2 - T - A^2 - Rk^2) U(\xi) = 0$$

finally, the equation can be simplified as:

$$\frac{d^2 U(\xi)}{d\xi^2} + RS U^3(\xi) + \nu U(\xi) = 0$$

where $\nu = Rk^2 - RT - RA^2 - R^2k^2$. Applying now the $G'/G$-expansion method to Eq. (20), we first have to
By using Eq. (23) and Eq. (21) in Eq. (20), we obtain the following polynomial sorted in terms of $\chi$

\[ a_1 \lambda \mu + RSa_0^3 + \nu a_0 + (a_1(\lambda^2 + 2\mu) + 3RSA_0^2a_1 + \nu a_1) \chi + (3a_1\lambda + 3RSA_0a_1^2) \chi^2 + (2a_1 + RSA_1^3) \chi^3 = 0 \quad (24) \]

Equation (24) is fulfilled when the coefficients of the polynomial are taken to zero, thus we end up with a system of 4 equations:

\[ \begin{align*}
    a_1 \lambda \mu + RSa_0^3 + \nu a_0 &= 0 \\
    a_1(\lambda^2 + 2\mu) + 3RSA_0^2a_1 + \nu a_1 &= 0 \\
    3a_1\lambda + 3RSA_0a_1^2 &= 0 \\
    2a_1 + RSA_1^3 &= 0
\end{align*} \quad (25) \]

The corresponding set of solutions are:

Solution 1) Trivial solution:

\[ a_1 = 0 = a_0 \quad \text{or} \quad a_1 = 0 \quad \text{for any } a_0 \text{ constant} \quad (26) \]

All remaining solutions are non-trivial with $a_1 \neq 0$.

Solution 2)

\[ \begin{align*}
    a_1 &= \pm i \sqrt{\frac{2}{RS}} \\
    a_0 &= -6^{\frac{1}{3}}\nu + \left( \mp 9i\lambda \mu + \sqrt{6\nu^3 - 81\lambda^2\mu^2} \right)^{\frac{2}{3}} \\
\end{align*} \quad (27) \]

Solution 3)

\[ \begin{align*}
    a_1 &= \pm i \sqrt{\frac{2}{RS}} \\
    a_0 &= -\sqrt{24\nu} + (-2)^{\frac{1}{3}} \left( \mp 9i\lambda \mu + \sqrt{6\nu^3 - 81\lambda^2\mu^2} \right)^{\frac{2}{3}} \\
\end{align*} \quad (28) \]
Figure 5. Harmonic solutions of the NLS equation with $\lambda^2 - 4\mu < 0$ and $c_1 < c_2$. The parameters used to obtain these solutions are: $R=-2$, $S=T=A=1$, $\lambda = 2$, $\mu = 3$, $c_1 = 2$, $c_2 = 5$ and $k=0.25$. a) 3D plot of the harmonic solution. $|\phi|^2$ is plotted in the range from 0 up to 15. b) Same plot as in a) but just for $t=20$.

Figure 6. Harmonic solutions of the NLS equation with $\lambda^2 - 4\mu < 0$ and $c_1 > c_2$. The parameters used to obtain these solutions are: $R=-2$, $S=A=1$, $T=-51$, $\lambda = 2$, $\mu = 3$, $c_1 = 50$, $c_2 = 2$ and $k=0.25$. a) 3D plot of the harmonic solution. $|\phi|^2$ is plotted in the range from 0 up to 100. b) Same plot as in a) but just for $t=20$.

Solution 4)

\[
\begin{align*}
    a_1 &= \pm i \sqrt{\frac{2}{RS}} \\
    a_0 &= \frac{-\sqrt{6}\nu + (\mp 9i\lambda \mu + \sqrt{(6i\nu^3 - 81\lambda^2\mu^2)})^{\frac{1}{3}}}{2^{\frac{1}{3}}3^{\frac{1}{3}}\sqrt{RS}} \left( \mp 9i\lambda \mu + \sqrt{(6i\nu^3 - 81\lambda^2\mu^2)} \right)^{\frac{1}{3}} 
\end{align*}
\]

Solution 6)

\[
\begin{align*}
    a_1 &= \pm i \sqrt{\frac{2}{RS}} \\
    a_0 &= \pm \lambda \sqrt{\frac{\lambda \mu}{2RS}} 
\end{align*}
\]

The general solution of Eq. (22) is:

a) Case 1: Self-focusing solution ($\lambda^2 - 4\mu > 0$)

\[
\chi(\xi) = \frac{\sqrt{\lambda^2 - 4\mu}}{2} \left( \frac{c_1 \cosh \left( \frac{\sqrt{\lambda^2 - 4\mu}}{2} \xi \right) + c_2 \sinh \left( \frac{\sqrt{\lambda^2 - 4\mu}}{2} \xi \right)}{c_2 \cosh \left( \frac{\sqrt{\lambda^2 - 4\mu}}{2} \xi \right) + c_1 \sinh \left( \frac{\sqrt{\lambda^2 - 4\mu}}{2} \xi \right)} \right)
\]

b) Case 2: Periodic solution ($\lambda^2 - 4\mu < 0$)
\[ \chi(\xi) = \frac{\sqrt{4\mu - \lambda^2}}{2} \left( \frac{c_1 \cos \left( \frac{\sqrt{4\mu - \lambda^2}}{2} \xi \right) - c_2 \sin \left( \frac{\sqrt{4\mu - \lambda^2}}{2} \xi \right)} {c_2 \cos \left( \frac{\sqrt{4\mu - \lambda^2}}{2} \xi \right) - c_1 \sin \left( \frac{\sqrt{4\mu - \lambda^2}}{2} \xi \right)} \right) \]  

where \( c_1 \) and \( c_2 \) are arbitrary constants. Finally, the family of solutions for the one-dimensional extended time-dependent NLS equation (see Eq. (16)) are obtained after substituting Eqs. (32)-(33) in Eq. (21) with the constants \( a_0 \) and \( a_1 \) already calculated in Eqs. (26)-(31).

Some representative solutions of Eq. (16) are plotted in Figs. 3-6 for a different set of parameters. Thus, in Figs. 3-4 we plot the solitonic solutions for \( \lambda^2 - 4\mu > 0 \). The profile of the solution depends on the numerical value of the parameters but for the whole set of solutions, they can be classified in three different groups, i.e., kink, antikink and kink–anti-kind pairs. Notice the different solitonic profile shown in Fig. 4 with respect to Fig. 3 c). In the case of \( \lambda^2 - 4\mu < 0 \), we basically obtain the harmonic or periodic solutions. Particularly, in Figs. 5 b)-6 b), it can be appreciated the difference of both periodic profiles.

**APPENDIX B**

In order to detail on the time evolution of two localized Gaussian perturbations within extended NLS provided in Section V, we have performed a set of calculations with different initial parameters. We have analyzed the evolution of two localized Gaussian perturbations with the same parameters as described in Fig. 2 b) of Section V, except for the initial positions of the perturbations. We noticed that the attractive force gets weaker and the time period between two polaronic collisions larger as soon as the positions of the initial excitations are increasing in distance (Fig. 7 a)-b)). Finally, for the initial excitations located at sites \( n = -7 \) and \( n = 7 \), we obtained collisionless propagation during the time of numerical simulation (see Fig. 7 c)).

Next, we studied influence of a very minute change of the height of the potential \( V_p \). We performed evolution of the nonlocal solution for \( V_p=1.901 \) eV (Fig. 7 d)) and observed noticeable changes compared with Fig. 2 a) in the Section V, where the height of the potential is \( V_p=1.916 \) eV.

Finally, we performed the time evolution for the same parameters as described in Fig. 2 b) of Section V, except for the strength of the Pöschl-Teller potential. We noticed that reducing the strength of the Pöschl-Teller potential, the time over which both excitations are attracted is considerably diminished (Fig. 7 e)-f)).

**APPENDIX C**

Here we will demonstrate that the extended time-depend continuous NLS equation as described in Eq. (16) admits internal modes. The demonstration is based partially in Ref. [37]. In order to determine the internal mode, we first analyse small linear perturbations upon the soliton solution, \( \phi_0(x,\omega) \), of Eq. (16). Then, we linearise the extended time-dependent continuous NLS equation around the soliton solution applying the following ansatz:

\[ \phi(x,t) = (\phi_0 + (Y(x,\omega,\Omega) + Z(x,\omega,\Omega)))e^{-i\omega t} + (Y^*(x,\omega,\Omega) - Z^*(x,\omega,\Omega))e^{i\omega t} \]  

where \( Y \) and \( Z \) are complex functions, \( \Omega \) is an eigenvalue and \( \omega \) represents the frequency induced to the frequency of the fundamental wave. The asterisk stands for the complex conjugation. Substituting Eq. (34) in Eq. (16), neglecting nonlinear terms and also taking into account that the soliton solution \( \phi_0(x,\omega) \) satisfies the extended time-dependent continuous NLS, the problem described in Eq. (16) can be reduced to the following linear eigenvalue problem

\[ \begin{pmatrix} 0 & \hat{L}_0 \\ \hat{L}_1 & 0 \end{pmatrix} \begin{pmatrix} Y \\ Z \end{pmatrix} = \Omega \begin{pmatrix} Y \\ Z \end{pmatrix} \]  

where \( \hat{L}_0 = -R \frac{\partial^2}{\partial x^2} + \omega - 2S|\phi_0|^2 + S\phi_0^2 + T \) and \( \hat{L}_1 = -R \frac{\partial^2}{\partial x^2} + \omega - 2S|\phi_0|^2 - S\phi_0^2 + T \). By using the ansatz \( \phi = e^{i\lambda t} \), Eq. (16) can be recast in the form:

\[ R \frac{\partial^2 \tilde{\phi}}{\partial x^2} - \omega \tilde{\phi} + (S|\phi|^2 - T)\tilde{\phi} = 0 \]  

where \( \tilde{\phi} \) represents a general localised solution. Now, assuming the case with \( T \ll 1 \) in Eq. (16), we can perturbately expand the soliton solution as:

\[ \phi = \phi_0 + T\varphi_1 \]  

with \( \varphi_0, \varphi_1 \in \mathbb{R} \). Performing the expansion given by Eq. (37) in the operators \( \hat{L}_0 \) and \( \hat{L}_1 \) and neglecting terms in \( T^2 \) yields

\[ \hat{L}_0 = -R \frac{\partial^2}{\partial x^2} + \omega - 2ST\varphi_0\varphi_1 + T = \hat{L}_0^0 + T\hat{L}_1^1 \]  

\[ \hat{L}_1 = -R \frac{\partial^2}{\partial x^2} + \omega - 3S\varphi_0^2 - 6ST\varphi_0\varphi_1 + T = \hat{L}_0^1 + T\hat{L}_1^1 \]  

where \( \varphi_0 \) satisfies Eq. (36) with \( T=0 \) or equivalently, the equation \( \hat{L}_0^0 \varphi_0 = 0 \) while \( \varphi_1 \) is governed by the linear
inhomogeneous equation
\[ \hat{L}_0^1 \varphi_1 = -T \varphi_0 \] (38)

As already indicated in Refs. [37, 38], the internal mode is a localised solution of the perturbed eigenvalue problem
\[ \begin{pmatrix} 0 & \hat{L}_0^1 + T \hat{L}_1^1 \\ \hat{L}_1^0 + T \hat{L}_1^1 & 0 \end{pmatrix} \Phi_{in} = (\omega - T^2 \kappa^2) \Phi_{in} \] (39)

with \( \kappa \), a real parameter and the solution of the eigenvalue problem in Eq. (39) is given by the combination of the \( \psi^\pm \) functions as
\[ \Phi_{in}(x) = \int dx [f^+(\kappa) \psi^+(x, \kappa) + f^-(\kappa) \psi^-(x, \kappa)] \] (40)

where the \( f^+, f^- \) coefficients are given by orthogonality relations (see Ref. [37]) and the functions \( \psi^\pm = \begin{pmatrix} \psi_1^\pm \\ \psi_2^\pm \end{pmatrix} \) are eigenvectors of the following eigenvalue problem
\[ \begin{pmatrix} 0 & \hat{L}_1^0 \\ \hat{L}_1^1 & 0 \end{pmatrix} \psi^\pm = \pm (\omega + \kappa^2) \psi^\pm \] (41)

As already reported in Ref. [37], the condition for the existence of the internal mode is that \( \kappa > 0 \), where \( \kappa \) is calculated as
\[ \kappa = -\frac{1}{4} \int dx [\psi_1^+(-x, 0) \hat{L}_1^1 \psi^+_1(x, 0) + \psi_2^+(-x, 0) \hat{L}_0^1 \psi^+_2(x, 0)] \]

For a symmetric solution \( \psi^\pm \) and the conditions
\[ 2S \varphi_0 \varphi_1 > 1 \] (43)
\[ 6S \varphi_0 \varphi_1 > 1 \] (44)

the parameter \( \kappa \) becomes positive and then, the extended time-dependent NLSE provided by Eq. (16) admits internal modes.
[28] Supplementary material.