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We consider polarons in models of coupled electronic and vibrational degrees of freedom, in the presence of a soft nonlinear inter-particle potential (Morse potential). In particular, we focus on a a bound state of a polaron with a breather, a so-called "polarobreather". We analyze the existence of this branch based on frequency resonance conditions and illustrate its stability using Floquet spectrum techniques. Multi-site solutions of this type are also obtained both in the stationary case (two-site polarons) and in the breathing case (two-site polarobreathers). We also obtain a different branch of solutions, namely a polaronic nanopteron.

Keywords: Polarons; Discrete breathers; Polarobreathers

I. INTRODUCTION

In the past few years, the study of discrete nonlinear systems has received a lot of attention, chiefly due to the increasing number of pertinent physical applications [1]. Among the various areas of recent interest, one can highlight coupled waveguide arrays in nonlinear optics [2], Bose-Einstein condensates (BECs) trapped in deep optical lattices (OLs) [3] in atomic physics, coupled cantilever systems in nano-mechanics [4], the local denaturation of the DNA double strand in biophysics [5], stellar dynamics in astrophysics [6], and so on.

In the study of such discrete nonlinear systems, an important concept is the possibility of intrinsic localization due to interacting degrees of freedom, even in a linear regime, as proposed by Holstein [7, 8]. This type of systems has been shown to sustain single- and multi-humped polaronic and excitonic solutions [9]. The same notion of effective nonlinearity in the setting of coupled excitonic and vibrational degrees of freedom was central to Davydov's suggestion of solitonic excitations arising in biomolecules [10, 11]. More recently, a new aspect has been added to this type of problems [12, 13], by considering the interplay of the linear self-trapping with a soft nonlinear potential, such as a Morse potential. This has been proposed as a more general model relevant to many soft matter applications.

Our purpose in the present paper is to examine this type of model and to provide a number of insights regarding its solutions and their stability. We start by establishing that the main stationary solutions obtained in the earlier work of [12] (namely, the single-site polarons) are dynamically stable within their region of existence. We then turn our attention to a different class of solutions which are genuinely "breathing" in time and which will, thus, be termed *polarobreathers*. Such solutions were first obtained and discussed in the context of the Holstein model in [14, 15], from where this term is coined. Here, we will obtain (and justify, based on resonance conditions) the domain of existence of such solutions. We will also systematically investigate their stability, by performing the corresponding Floquet spectral analysis, and illustrate the existence of intervals of linear stability of these solutions. Our study of this new class of solutions will reveal yet another family of solutions consisting of a static polaron combined with a linear mode to give a form of polaronic nanopteron. Since the branch of stationary polarons terminates at a critical value of the coupling as illustrated in the earlier work of [12], we will examine the dynamics beyond this termination point with a single hump initial condition and will show that the solution develops large breathing fluctuations in its local (i.e., central site) energy in time due to an interplay between the central site of the localized profile and its neighbors. We will also highlight multi-site branches such as the two-site stationary solutions (polarons) and the two-site polarobreathers and numerically reveal their instability.

Our presentation will be structured as follows. In section II, we will present the model and numerical methods (the details of which are relegated to a technical appendix). Subsequently, in section III, we will present and discuss our numerical results. Finally, in section IV, we will summarize our conclusions and pose questions of interest for future studies.

II. THE MODEL

We consider the coupled charge/excitation-lattice model introduced in [12], describing the competition between linear polaronic self trapping and self-focusing effects of a soft nonlinear potential; in dimensionless form, it can be expressed as follows:

$$i\dot{\Psi}_n = -J(\Psi_{n+1} + \Psi_{n-1}) - \chi u_n \Psi_n, \quad (1)$$

$$\ddot{u}_n = -V'(u_n) + \chi|\Psi_n|^2 + k(u_{n+1} - 2u_n + u_{n-1}), \quad (2)$$

where dots denote time derivatives, and the lattice index n runs from 1 to N (the total number of lattice sites). In Eqs. (1)-(2), $\Psi_n(t)$ represents the "electronic" degrees of freedom, u_n corresponds to the lattice displacements (i.e., "vibrational" degrees of freedom), while the parameters J, k and χ denote, respectively, the transfer integral, the lattice spring constant and the coupling constant between the interacting fields. Finally, $V(u_n)$ is an anharmonic on-site potential, which, similarly to [12], is assumed to have the form of a Morse potential:

$$V(u) = \frac{1}{2}[\exp(-u) - 1]^2. \tag{3}$$

The dynamical equations (1)-(2) arise from the Hamiltonian:

$$\begin{aligned} H &= \sum_n \left[\frac{1}{2}\dot{u}_n^2 + V(u_n) + \frac{k}{2}(u_n - u_{n+1})^2\right] \\ &- \sum_n \left[\chi(|\Psi_n|^2 u_n) + J(\Psi_n \Psi_{n+1}^* + \text{c.c.})\right] \end{aligned} \tag{4}$$

We will seek standing-wave, as well as genuinely time-periodic solutions of Eqs. (1)-(2). To factor out the phase invariance of Eq. (1), and clearly separate between the two classes of solutions, we introduce the transformation:

$$\Xi_n(t) = \Psi_n(t)\mathrm{e}^{-i\omega_\mathrm{e} t}. \tag{5}$$

Then, the dynamical equations take the following form:

$$i\dot{\Xi}_n - \omega_\mathrm{e}\Xi_n + J(\Xi_{n+1} + \Xi_{n-1}) + \chi u_n \Xi_n = 0, \tag{6}$$
$$\ddot{u}_n + V'(u_n) - \chi|\Xi_n|^2 - k(u_{n+1} - 2u_n + u_{n-1}) = 0. \tag{7}$$

Stationary solutions now correspond to ones where all time derivatives in Eqs. (6)-(7) are set to zero. On the other hand, time periodic solutions are characterized by a frequency of oscillation ω_b (or period $T_\mathrm{b} = 2\pi/\omega_\mathrm{b}$) in the time dependence of both the electronic wavefunction Ξ_n and of the lattice displacements u_n. Our aim is to study the existence and stability of such stationary and breathing polaron solutions; the latter, adopting the terminology of [14, 15], will be henceforth called "polarobreathers". In the results to be presented below, we have fixed the values of the transfer integral and lattice spring constant, namely $J = 0.005$ and $k = 0.13$, and let the coupling constant χ and the polarobreather frequency ω_b vary. Nevertheless, in our study, we have also considered other parameter values (such as, e.g., $k = 0.065$, $k = 0.26$, $J = 0.0025$ and $J = 0.01$) and we have obtained qualitatively similar results to those reported below.

In order to find either stationary or time-periodic solutions of the dynamical equations (6)-(7), we use methods based on the anti-continuous limit [16, 17]. In particular, we first obtain a nontrivial steady state u_0 -for stationary solutions- or an orbit of frequency ω_b for an isolated oscillator $u_0(t)$-for time periodic solutions. Then, the solution at the anticontinuous limit ($k = J = \chi = 0$) is $\Xi_n = u_n = 0$, except at $n = 0$, which is set to u_0. The coupling constants are subsequently varied through a path-following (Newton-Raphson) method. In the following, we first vary χ up to 0.02, then J up to 0.005 and, finally, k up to 0.13. Once J and k are fixed, χ can be freely varied. The implementation of the anticontinuous limit has been performed in real space (using a shooting method) and in Fourier space. Note that the first method is less accurate than the second one, whereas the latter is rather time consuming, particularly in the case of long chains. We have made use of both methods in the calculations presented herein.

Once the numerically exact [up to the prescribed accuracy $\mathrm{O}(10^{-7})$] solutions are obtained, linear stability analysis is performed to examine the dynamical stability of the solutions. In the case of stationary solutions, this is implemented by imposing normal mode perturbations (see, e.g., earlier work in [8, 13, 18]) and obtaining the corresponding eigenvalues of the ensuing linear matrix problem. On the other hand, in the case of (time-periodic) polarobreather solutions, we impose time-dependent perturbations to both the electronic and vibrational fields and solve the resulting (linear) differential equations for the perturbations from $t = 0$ to $t = T_b$. Then, obtaining the Floquet (or monodromy) matrix, which relates the perturbation vector at $t = 0$ to that at $t = T_b$, we compute the Floquet multipliers of the periodic solution. The Floquet multipliers imply stability (instability), if they do (do not) appear only on the unit circle. The details of the numerical methods used in this work are discussed in the Appendix.

III. NUMERICAL RESULTS

In this section we illustrate the numerical results obtained for the polarobreathers. Recall that in all calculations we have fixed $J = 0.005$ and $k = 0.13$, χ being a free parameter.

We first consider the stability of static polarons. Such polarons, localized on a single lattice site, are stable. Considering perturbations of these structures, namely $u_n(0) = u_n^0(0) + \varepsilon\delta_{n,0}$ and $Re(\Psi_n(0)) = Re(\Psi_n^0(0)) + \varepsilon\delta_{n,0}$ (where the zero superscript denotes an exact solution), it is found that the polaron evolves into a vibrating state, which is a normal mode of the system. This result is clearly illustrated in Fig. 1 (here we have used $\varepsilon = 0.001$ and $\chi = 0.5$); note that in the relevant Fourier spectrum (right panels of the same figure for the vibrational (top) and electronic (bottom) field at the central site), there appears a single excited frequency.

Apart from static polarons, there exist stable, time-periodic and spatially localized solutions within the context of the model, namely *polarobreathers*. Fig. 2 shows an example of these solutions along with the relevant Floquet spectrum. Additionally, Fig. 3 shows the Fourier spectrum of this solution, whose nonlinear character implies the existence of integer multiples of its frequency.

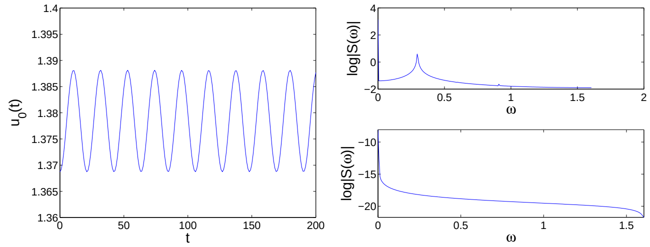

FIG. 1: Left panel: Evolution of the displacement of the central particle of a slightly perturbed static polaron with $\chi = 0.5$ Right panels: The Fourier spectrum of the corresponding time series is shown (the top part corresponds to the lattice variable and the bottom part to the electronic one). The existence of only one frequency indicates the simple periodic nature of the solution.

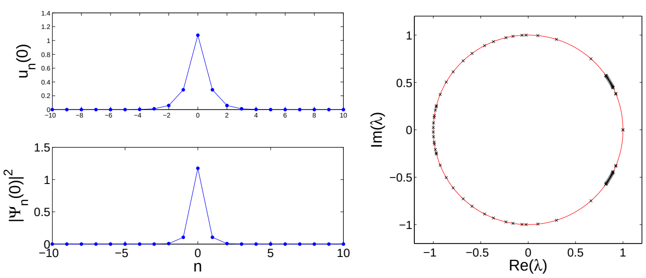

FIG. 2: Left panels: Profiles of the lattice (u_n, top) and electronic component ($|\Psi_n|^2$, bottom) of a polarobreather with $\omega_\mathrm{b} = 0.8$ and $\chi = 0.15$. Right panel: Floquet spectrum of this solution.

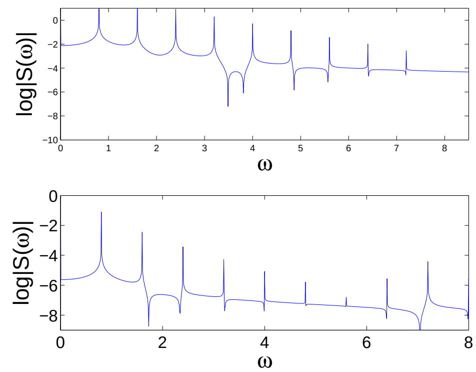

FIG. 3: Fourier spectrum of the polarobreather of Fig. 2. The top and bottom panels correspond to the lattice and electronic variables respectively.

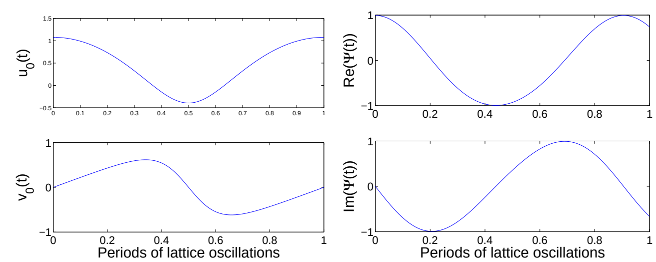

FIG. 4: Time evolution of the lattice (left panel) and electronic coordinates (right panel) of a polarobreather with $\omega_\mathrm{b} = 0.8$ and $\chi = 0.15$. Notice that the oscillation period of the two functions is different.

The time evolution of the lattice ($u_0(t)$) and electronic ($\Psi_0(t)$) variables of the central particle is displayed in Fig. 4. Notice the different period in the oscillation of the u and the Ψ fields, due to the additional inclusion, in the latter, of the oscillation with frequency ω_e. Polarobreathers exist as long as the conditions of the MacKay-Aubry's theorem [16] are fulfilled, i.e., none of the harmonics of the polarobreather frequency resonate with the linear modes. Based on this criterion, an analysis of the linear modes can provide the range of existence of polarobreathers of a given frequency. Fig. 5 shows the real part of the normal mode frequencies and indicates the existence of a continuum band of (extended) linear modes besides several localized modes. Since we are dealing with polarobreathers in a soft potential, they must stem from the linear mode at the bottom of the band of extended modes. This mode becomes localized (i.e., bifurcates from the continuous spectrum band) at the value of $\chi \approx 0.033$ and its location varies with χ. As a result, the polarobreather frequency must be smaller than this localized-mode frequency. This fact is indicated in the right panel of Fig. 5. It can be the observed that the bifurcation points correspond to the values of χ for which the frequency of the localized mode coincides with the frequency of the polarobreather branch.

The existence of polarobreathers is also limited by the second-harmonic resonances. In the case of finite lattices, "phantom" solutions can appear due to the existence of gaps in the extended modes band [19]. These solutions consist of a core that vibrates with the fundamental frequency ω_b (or may also be static), whereas the tails correspond to a phonon vibrating with frequency $2\omega_\mathrm{b}$. These solutions are an artifact of the finiteness of the lattice and, moreover, they are usually unstable. An example of a phantom polarobreather is shown in Fig. 6 (for $\omega_\mathrm{b} = 0.6$ and $\chi = 0.15$).

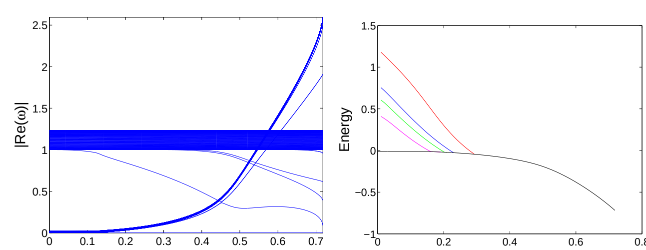

FIG. 5: The left panel shows the real part of the linear mode spectrum. The right panel shows the dependence of the polarobreather energy as a function of χ for different values of the frequency (from left to right): $\omega_\mathrm{b} = 0.9, 0.84, 0.8, 0.7$. The line at the bottom corresponds to the static polaron.

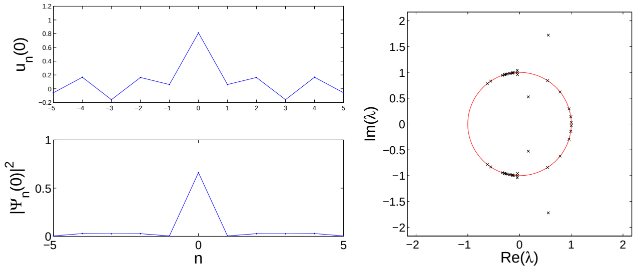

FIG. 6: Left panels: The profiles of the lattice (top) and the electronic (bottom) components of a phantom polarobreather are shown for $\omega_{\rm b} = 0.6$ and $\chi = 0.15$. Right panel: Floquet spectrum of this solution.

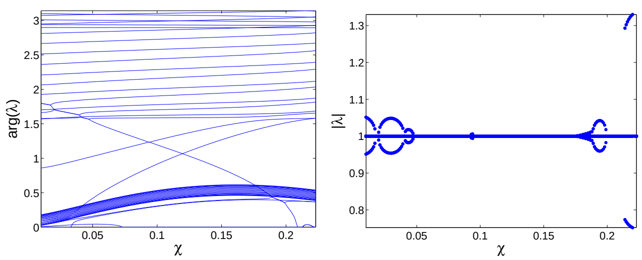

FIG. 7: The argument (left) and modulus (right) of the Floquet eigenvalues as a function of the coupling constant χ for one-site polarons.

An analysis of the stability of polarobreathers is shown in Fig. 7. It is observed that, for the considered branch, the only kind of instabilities that arise are oscillatory ones (stemming from complex Floquet multipliers). The small growth rate of the ensuing instabilities, however, renders the polarobreathers relatively long-lived metastable structures when they are not linearly stable.

Apart from one-site (site-centered) polarons, we have also considered two-site (bond-centered) static polarons and polarobreathers. Whereas one-site polarons are stable, two-site ones are unstable. An example is shown in Fig. 8, where the real and imaginary parts of the linear mode spectrum for two-site polarons are illustrated.

Similarly to their static counterparts, two-site polarobreathers are unstable. This instability can be either exponential (i.e., the Floquet eigenvalues responsible for

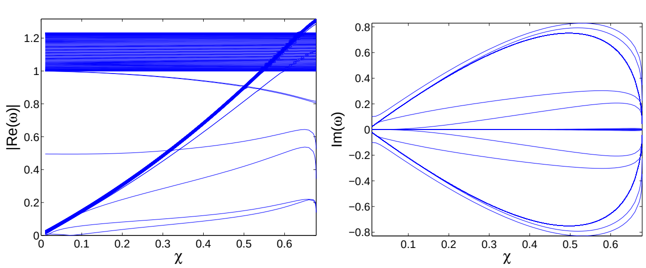

FIG. 8: The real (left) and imaginary (right) part of the linear mode spectrum as a function of the coupling constant χ for two-site polarons.

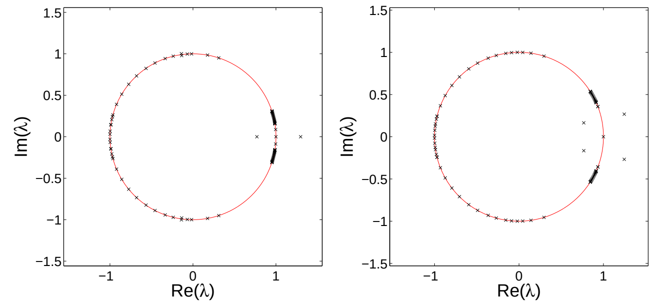

FIG. 9: Floquet spectra for a two-site polarobreather, subject to a harmonic (left panel, $\chi = 0.5$) or an oscillatory (right panel, $\chi = 0.15$) instability.

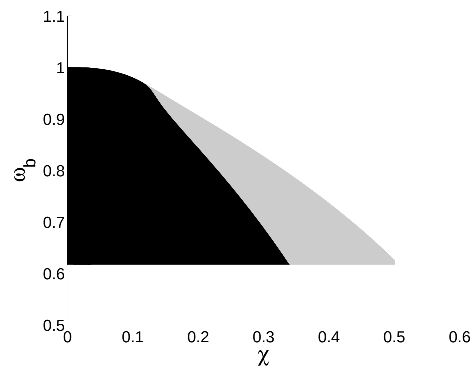

FIG. 10: Domain of existence of one-site (black region) and two-site (black *and* gray region) polarobreathers in the χ-$\omega_{\rm b}$ parameter plane.

the instability have zero phase) for small χ, or oscillatory (i.e., the Floquet eigenvalues responsible for the instability have phases different from zero or π). In Fig. 9, examples of the Floquet spectra pertaining to a regular exponential (for $\chi = 0.5$) and an oscillatory instability (for $\chi = 0.15$) are shown.

Two-site polarobreathers can be continued as a function of χ for J and k fixed. As in the one-site case, the branches for a fixed frequency merge with a static solution branch. The domains of existence of the one-site and two-site polarobreathers for $k = 0.13$ and $J = 0.005$ are shown in Fig. 10. It is interesting to note that, similarly to what happens for their static counterparts [12], one-site polarobreathers have a narrower domain of existence (gray region in Fig. 10) than their two-site counterparts (gray and black region in Fig. 10). Given that the termination of such branches occurs upon their collision with the stationary branch of solutions, this trait is rather natural to expect in the present setting. A wider domain of existence for two-site breathers was also observed in a model with competing attractive and repulsive interaction [20].

In order to examine the dynamical evolution of the instability of two-site polarons, we again consider the perturbation $u_n(0) = u_n^0(0) + \varepsilon\delta_{n,0}$ and $Re(\Psi_n(0)) = Re(\Psi_n^0(0)) + \varepsilon\delta_{n,0}$, with the value $\varepsilon = 0.001$ pertaining

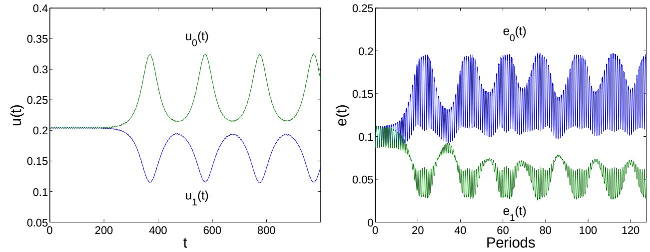

FIG. 11: Evolution of the central particles displacements and energy densities, respectively, for a perturbed two-site polaron with $\chi = 0.35$ (left panel) and a two-site polarobreather with $\chi = 0.2$ (right panel).

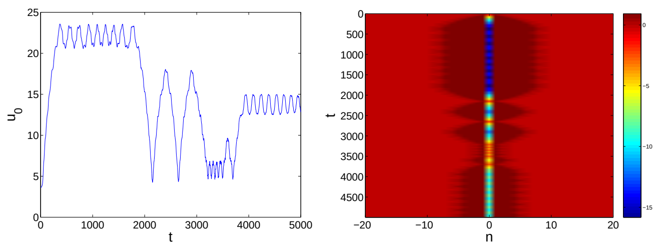

FIG. 12: (Color online) Left panel: Time evolution of the displacement of the central particle at $\chi = 0.72$ using as initial condition a static polaron at $\chi = 0.718$. Right panel: the energy density plot.

to a static polaron. It can be observed that, as illustrated in Fig. 11, after a transient, the polaron evolves into an anti-phase vibrating state; note that if the two central particles were perturbed, the observed behaviour would be similar, but the transient would be longer. If the same perturbation is applied to a two-site polarobreather, the behavior is somewhat reminiscent of that observed for a static polaron. This is illustrated in Fig. 11 by displaying the temporal evolution of the energy density at the two principal sites of the solution. The energy density is defined as:

$$\begin{aligned} e_n &= \frac{1}{2}\dot{u}_n^2 + V(u_n) + \frac{k}{4}\left[(u_n - u_{n+1})^2 + (u_n - u_{n-1})^2\right] \\ &- \chi|\Psi_n|^2 u_n - \frac{J}{2}(\Psi_n(\Psi_{n+1}^* + \Psi_{n-1}^*) + \text{c.c.}) \qquad (8) \end{aligned}$$

Another interesting fact is that the static polaron branch does not exist for $\chi > \chi_c \approx 0.718$. In particular, if the solution for a polaron close to χ_c is used as initial condition for $\chi > \chi_c$), e.g., for $\chi = 0.72$, we have found the following type of evolution (see figure 12): first, for some finite time, a continuous increase of the "local" energy at the central site of the solution occurs (coupled to a corresponding decrease in the energy of the immediate neighboring sites). Then, the system "relaxes" so that a quasi-breathing evolution of the energy density is observed; however, its strong localization at the central site of the lattice is essentially preserved for long times.

IV. CONCLUSIONS

In this work, we have discussed the existence and stability of localized solutions in a generalized Holstein model with a soft (Morse-type) inter-particle potential. We have shown that in addition to the standard stationary polaronic solutions within this model discussed elsewhere [12], there exists also very robust breathing behavior in the form of a time-periodic type of state: the polarobreather solutions. Using Floquet analysis, we have illustrated the existence of parametric intervals of stability of the latter solutions, and we have also elucidated their domain of existence based on resonance conditions. In this respect, we have shown that the polarobreathers cease to exist as a result of their "collision" with the standard polaronic branch, occurring at frequency-dependent values of the relevant coupling parameter. We have also found that "phantom" versions of such polarobreathers exist in finite lattices but are usually unstable. We can view these dressed polaron solutions as "hot" polarons (or excitons in related exciton-vibron systems). However, the polarobreather is dressed with a coherent phonon wavepacket (a breather), which binds with the polaron as a composite local excitation. We have also obtained multi-site polarons (such as the two-site polarons examined herein) and multi-site polarobreathers (such as the two-site polarobreathers, also studied herein), and numerically demonstrated their instability. Finally, we have shown that the unstable polaronic dynamics (for parameter values beyond the range of existence of their corresponding stationary branch) may lead to energy redistribution and eventual oscillatory dynamics for longer timescales.

It is interesting to examine higher-dimensional generalizations of the model and the possibility for obtaining localized solitary wave or vortex-like solutions in such higher-dimensional discrete contexts. Such studies are currently in progress and will be reported elsewhere. It would also be important to assess the significance of quantum effects in both the electronic and lattice degrees of freedom. Initial results [21] suggest that bound states of breathers and polarons (or excitons) may indeed persist in appropriate regimes.

V. APPENDIX: DETAILS OF NUMERICAL METHODS

A. Real space methods

In order to analyze Eqs. (6)-(7) using the real space method, it is convenient to separate the electronic wavefunction into its real and imaginary part, $\Xi_n(t) = \phi_n(t) + i\varphi_n(t)$, and also define the oscillation velocity $v_n(t) = \dot{u}_n(t)$. In this way, we end up with a system of $4N$ equations (N is the number of particles of the system):

$$\begin{aligned}\dot{\phi}_n &= -(-\omega_\mathrm{e} + \chi u_n)\varphi_n - J(\varphi_{n+1} + \varphi_{n-1}),\\ \dot{\varphi}_n &= (-\omega_\mathrm{e} + \chi u_n)\phi_n - J(\phi_{n+1} + \phi_{n-1}),\\ \dot{u}_n &= v_n,\\ \dot{v}_n &= -V'(u_n) + \chi(\phi_n^2 + \varphi_n^2)\\ &+ k(u_{n+1} - 2u_n + u_{n-1}). \end{aligned} \tag{9}$$

Then, if we define $X(t) \equiv \{u_n(t), v_n(t), \phi_n(t), \varphi_n\}$, there exists a map $\mathcal{T}$ which relates $X(0)$ and $X(T_\mathrm{b})$ as $X(T_\mathrm{b}) = \mathcal{T}X(0)$. The shooting (real space) method consists in finding zeros of the map $F \equiv \mathcal{T}X(0) - X(T_\mathrm{b})$ [14] (for a detailed explanation of the shooting method, see [22]). The tangent map needed for the application of the Newton method, $J \equiv \partial\mathcal{T}$, must be calculated numerically.

However, in this scheme the electronic norm is not conserved and the electronic frequency ω_e must be known. For this reason, an equation is added to (9),

$$\sum_n(\phi_n^2 + \varphi_n^2) - 1 = 0, \tag{10}$$

so that the norm is conserved, and a new variable ω_e is added to the vector $X(t)$.

B. Fourier space methods

The Fourier space methods (see details in [23, 24]) are based on the fact that both the electronic wavefunction and the lattice displacements are periodic with period T_b. Thus, they can be expressed in terms of a truncated Fourier series expansion:

$$\begin{aligned}\Xi_n(t) &= \sum_{k=-k_m}^{k_m} a_n^k \exp(ik\omega_\mathrm{b}t),\\ u_n(t) &= \sum_{k=-k_m}^{k_m} b_n^k \exp(ik\omega_\mathrm{b}t).\end{aligned} \tag{11}$$

Then, the dynamical equations (6)-(7) are reduced to a set of $(2N+1)\times(2k_m+1)$ algebraic equations (we have also included the norm conservation), where the variables are $Z \equiv \{a_n^k, b_n^k, \omega_\mathrm{e}\}$:

$$\begin{aligned}F_{E,n}^k &\equiv -\omega_\mathrm{b}ka_n^k - \omega_\mathrm{e}a_n^k + \mathcal{F}^k(V'(u_n)) + \chi\mathcal{F}^k(u_n\Xi_n)\\ &+ J(a_{n-1}^k + b_{n+1}^k) = 0,\\ F_{B,n}^k &\equiv -\omega_\mathrm{b}^2k^2b_n^k + \mathcal{F}^k(V'(u_n)) - \chi\mathcal{F}^k(|\Xi_n|^2)\\ &- k(b_{n-1}^k - 2b_n^k + b_{n+1}^k) = 0\\ F_{N,n} &\equiv (\sum_n\sum_k\sum_{k'} a_n^k a_n^{k'}) - 1 = 0.\end{aligned} \tag{12}$$

In the above equations, $\mathcal{F}^k$ denotes the Discrete Fourier Transform:

$$\mathcal{F}^k(u) = \sum_{j=-k_m}^{k_m} u(t_j)\exp(ik\omega_\mathrm{b}t_j), \tag{13}$$

where t_j is a sample of times that must be equally spaced according to

$$t_j = \frac{2\pi j}{\omega_\mathrm{b}(2k_m+1)}, \qquad j = -k_m, \dots, +k_m, \tag{14}$$

and $u(t_j)$ is calculated from the Fourier coefficients b^k by means of the Inverse Discrete Fourier Transform:

$$u(t_j) = \sum_{k=-k_m}^{k_m} b^k \exp(ik\omega_\mathrm{b}t_j). \tag{15}$$

The Newton operator or Jacobian $J \equiv \partial F$ (with $F \equiv \{F_{P,n}^k; F_{B,n}^k; F_N\}$ can be calculated analytically. One of the main disadvantages of this method is that the Jacobian is singular. Polarobreathers must be calculated using singular value decomposition [25]. However, this method allows the calculation of non-time-reversible solutions.

C. Normal modes and linear stability analysis

Here, we present the normal modes and stability equations, which were used in the results presented in the main text.

1. *Stationary Solution Stability: Normal modes*

In order to calculate the normal modes we first need to calculate a stationary polaron from Eqs. (1)-(2) from the following conditions [12]:

$$\begin{aligned}\Psi_n(t) &= \psi_n \exp(-i\omega_\mathrm{e}t),\\ \ddot{u}_n(t) &= \dot{u}_n(t) = 0.\end{aligned} \tag{16}$$

Then, the polaron is determined by the electronic wavefunction ψ_n and the lattice displacements y_n.

The normal modes are introduced as perturbations to a stationary polaron [8, 13, 18]:

$$\begin{aligned}\Psi_n(t) &= [\psi_n + \epsilon_n(t)]\exp(-i\omega_\mathrm{e}t),\\ u_n(t) &= y_n + \xi_n(t),\\ \dot{u}_n(t) &= \dot{y}_n + \pi_n(t) = \pi_n(t),\end{aligned} \tag{17}$$

and the dynamical equations for the normal modes are:

$$\begin{aligned}i\dot{\epsilon}_n &= -\omega_\mathrm{e}\epsilon_n - \chi(y_n\epsilon_n + \psi_n\xi_n) - J(\epsilon_{n+1} + \epsilon_{n-1}),\\ \dot{\xi}_n &= \pi_n,\\ \dot{\pi}_n &= -V''(y_n)\xi_n + \chi\psi_n(\epsilon_n + \epsilon_n^*),\\ &+ k(\xi_{n+1} - 2\xi_n + \xi_{n-1}).\end{aligned} \tag{18}$$

Normal mode frequencies can be calculated using the following relations:

$$\begin{aligned}\epsilon_n(t) &= a_n\exp(i\omega t) + b_n\exp(-i\omega^*t)\\ \xi_n(t) &= c_n\exp(i\omega t) + c_n^*\exp(-i\omega^*t)\\ \pi_n(t) &= d_n\exp(i\omega t) + d_n^*\exp(-i\omega^*t).\end{aligned} \tag{19}$$

Thus, the normal modes are determined by the following linear system:

$$\begin{aligned}
\omega a_n &= \omega_e a_n + \chi(y_n a_n + \psi_n c_n) + J(a_{n+1} + a_{n-1}), \\
\omega b_n^* &= -\omega_e b_n^* - \chi(y_n b_n^* + \psi_n c_n) - J(b_{n+1}^* + b_{n-1}^*), \\
\omega c_n &= -i d_n, \\
\omega d_n &= i[V''(y_n) c_n - \chi \psi_n (a_n + b_n^*) \\
&+ k(c_{n+1} - 2c_n + c_{n-1})]. \qquad (20)
\end{aligned}$$

As the normal mode operator is non-Hermitian, the frequencies are in general complex numbers. If non-real frequencies exist in the spectrum, then the stationary polaron is unstable.

2. Polarobreather Stability: Floquet Spectrum

Linear stability can be studied via a Floquet analysis. This analysis is performed by linearizing the dynamical equations around a polarobreather. Then, the analysis performed for the normal modes cannot be extended to the stability, as the electronic wavefunction does not possess gauge invariance. Thus, we introduce a perturbation $\Omega \equiv \{\alpha_n, \beta_n, \xi_n, \pi_n\}$ to Eqs. (9), which has the form:

$$\phi_n = \phi_n^0 + \alpha_n,\ \varphi_n = \varphi_n^0 + \beta_n,\ u_n = u_n^0 + \xi_n,\ \pi_n = \dot{\xi}_n, \qquad (21)$$

where the superscript zero denotes the polarobreather solution. Then, to leading-order approximation (i.e., keeping only the linear terms), the stability equations are:

$$\begin{aligned}
\dot{\alpha}_n &= -(-\omega_e + \chi u_n^0)\beta_n - \chi \varphi_n^0 \xi_n - J(\alpha_{n+1} + \alpha_{n-1}), \\
\dot{\beta}_n &= (-\omega_e + \chi u_n^0)\alpha_n + \chi \phi_n^0 \xi_n + J(\beta_{n+1} + \beta_{n-1}), \\
\dot{\xi}_n &= \pi_n, \\
\dot{\pi}_n &= 2\chi(\phi_n^0 \alpha_n + \varphi_n^0 \beta_n) - V''(u_n^0) \\
&- k(\xi_{n+1} - 2\xi_n + \xi_{n-1}). \qquad (22)
\end{aligned}$$

The Floquet operator (or monodromy matrix) $\mathcal{M}$ relates the vector Ω at $t = 0$ and $t = T_b$ as follows:

$$\Omega(T_b) = \mathcal{M}\Omega(0). \qquad (23)$$

A polarobreather is stable if all the eigenvalues of the monodromy matrix lie on the unit circle [15].

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