Soliton metacrystals: topology and chirality

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Designing metamaterials with the required band structure, topology and chirality using nanofabrication technology revolutionises modern science and impacts daily life. The approach of this work is, however, different. We take a periodic sequence, i.e., metacrystal, of the dissipative optical solitons rotating in a single ring microresonator and demonstrate its properties as of the electromagnetic metamaterial acting in the radio to terahertz frequency range. The metacrystal unit cell consists of the bound pair of solitons, and the distance between them is used as a control parameter. We are reporting the soliton metacrystal band structure and its topological properties. The latter is confirmed by the existence of the π steps experienced by the crystal phonons’ geometrical (Zak) phase. Furthermore, we found the phononic edge states in the metacrystals with defects made by removing several solitons. Optical frequency combs corresponding to the soliton metacrystals reveal the spectral butterfly pattern serving as a signature of the spatio-temporal chirality and bearing a resemblance to the butterfly wings illustrating natural occurrences of chirality.

RESULTS AND DISCUSSION

Two prolific themes spanning across today’s solid-state, cold-atom and optical physics are the topology of waves in periodic potentials [1–7] and localised coherent states, such as, e.g., solitons and vortices. The recent and ongoing work on the vortex and skyrmion matter and light, soliton crystals [2–19] and soliton gas [20, 21] points at the opportunity of using the localised structures of the coherent light and matter waves for designing new electromagnetic materials. Here, we present the proof-of-concept results revealing the topological properties of the periodic soliton sequences, i.e., soliton metacrystals, generated in optical microresonators.

For this work, we should distinguish the dissipative and conservative optical solitons and single out the former for their robustness and longevity [22]. Crystals of dissipative optical solitons are known to exist in Kerr ring microresonators [14–18], fibre lasers [23, 24], and in the exciton-polariton resonators [25]. Methods of the on-demand positioning of the individual dissipative solitons, circling with the typical repetition rates between ten GHz and one THz, inside the ring resonators have also been successfully demonstrated. These methods included pump modulation [16], using bi-chromatic pump [19], single pump frequency tuning [26], and the excitation of the desired soliton ordering by applying a sequence of pulses with the repetition rate higher than the resonator free spectral range [27]. Though the soliton crystals in optical resonators are well established, their band structure and its topology remain an uncharted territory.

The focus of many prior studies of topological properties of nonlinear optical systems has been on the cases when taking the no-nonlinearity limit leaves a linear system prepossessing a specially designed linear periodic structure, see, e.g., [28–32] for topological solitons and [33–34] for other topology vs nonlinearity interplay in the arrays of optical resonators and waveguides, and photonic crystals. The soliton crystals studied below require only a single optical resonator and are sustained by the pump-loss and dispersion-nonlinearity balances.

In this work, we demonstrate the soliton metacrystals consisting of the bound soliton pairs so that the soliton arrangement looks like the famous Su-Schrieffer-Heeger (SSH) lattice [4]. The relative positioning of the solitons within a unit cell is used as the control parameter helping to reveal topological and chiral properties. To prove the non-trivial topology of the metacrystal band structure, we develop a theory of their geometrical phase [43, 44], and also demonstrate the topological edge states [4] in the metacrystals with defects. The edge states typically come in chiral pairs as, e.g., the edge currents on the opposite interfaces of the suitably cut two-dimensional topological crystal [3, 4]. A feature of the multimode resonators is that the trains of the modelocked solitons they generate are periodic in space and time. We found that the spatio-temporal chirality of the soliton metacrystals leads to the distinct butterfly-like structure hidden in their optical spectra. Various practical and conceptual realizations of time crystals in condensed matter and optics [45–51] and the cross-disciplinary applications of chirality [52–55] are currently attracting the increasing attention.

Band structure of soliton metacrystals

We consider an optical ring microresonator [14] which frequency spectrum is approximated by \( \omega_\mu = \omega_0 + D_1 \mu + D_2 \mu^2/2! + D_3 \mu^3/3! \), where \( \mu = 0, \pm 1, \pm 2, \ldots \) is the mode number, \( D_1 \) is the linear repetition rate (inverse of the round-trip time), and \( D_2, D_3 \) are the second and third order dispersion coefficients. \( \omega_\mu \) typically belong to the infrared-to-visible range. The pump laser frequency \( \omega_p \) is tuned around \( \omega_0 \), so that \( \delta = \omega_0 - \omega_p \) is the detuning parameter. The envelope, \( \phi \), of the multimode
The middle panel shows how two solitons are positioned in the unit cell for varying separation distance, $S_n$. Two side panels show all $2K = 48$ solitons along the ring circumference. The right plot corresponds to $S_A = S_B$, i.e., when the molecular crystal degenerates to the atomic one. The left plot shows the molecular metacrystal and illustrates the two dimerization choices applied in this work, $S_A + S_B = 2\pi/K$. The scaled dispersion and detuning parameters are $d_2/\kappa = 5 \times 10^{-4}$, $d_3/\kappa = 5 \times 10^{-7}$, and $\delta/\kappa = 30$. The crystal repetition rates vary with $S_n$, but $d_1/\kappa$ remains close to $-0.01059$. The dimensionless field amplitude, $\psi$, is expressed as $\gamma|\psi|^2/\kappa = |\psi|^2$. The dimensionless pump parameter is $\gamma h^2/\kappa = 25$. Crystals are computed with 512 points across the unit cell, $\theta \in [0, 2\pi/K)$.

The difference of the interaction strengths between the left and right neighbours of a given soliton, in other words, the imbalance of the intra-cell and inter-cell coupling rates, is controlled by the separation distance $S_n$. There exist two choices of $S_n$, i.e., dimerization choices, corresponding to the same crystal, $S_n = S_A$ and $S_n = S_B = 2\pi/K - S_A$ (see Fig. 1). In what follows, we take $\pi/K < S_A < 2\pi/K$ and $0 < S_B < \pi/K$, so that the choice of the unit-cell $A$, i.e., dimerization $A$, corresponds to the inter-cell coupling being stronger than the intra-cell one. $S_{A,B} = \pi/K$ is the degeneracy point with equal coupling rates.

Soliton metacrystals should modify the spectrum of small amplitude perturbations, i.e., elementary excitations, supported by the resonator. Physically, these excitations are slow modulations of the amplitudes and phases of the resonator modes having frequencies in the radio- to tera-hertz range. Using an analogy with the density waves in the solid state crystals, we term these excitations - phonons. While the nonlinear interactions between the crystal and phonon modes are imperative in what follows, phonon to phonon interactions are weak and should be disregarded.

The phonon band structure is computed using the Bloch theorem. This is achieved by taking a soliton crystal, Eq. (2), and its complex conjugate, and representing the phonon field by the cell-periodic two-component...
Every Bloch vector is characterised by (i) Bloch momentum, \( k \), which can be restricted to the first Brillouin zone, \( k = 1, 2, \ldots, K \), (ii) band index, \( n \), and (iii) dimerization index, \( \alpha = A, B \). \( \beta_{k,n} = \beta_{k+K,n} \) are the phonon frequencies and \( \lambda_{k,n} = \lambda_{k+K,n} \) express the balance between the dissipation and parametric gain. The momentum varies discretely because of the ring geometry. The condition of the crystal stability, \( \lambda_{k,n} \leq 0 \), is satisfied for all solutions shown in Fig. 1. Below we use the ket notation for \( \mathbf{u}_{k,n}^{(\alpha)} = \left\{ u_{k,n}^{(\alpha)} \right\} \) and bra for its transpose and complex conjugate, \( \hat{\sigma}_x \mathbf{u}_{k,n}^{(\alpha)} = \langle \mathbf{u}_{k,n}^{(\alpha)} \rangle \).

The Bloch states solve the eigenvalue problem

\[
\hat{\sigma}_z \hat{H}_k^{(\alpha)} \mathbf{u}_{k,n}^{(\alpha)} = (\beta_{k,n} + i\lambda_{k,n} + i\frac{1}{2} \kappa) \mathbf{u}_{k,n}^{(\alpha)}, \quad \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},
\]

where \( \hat{H}_k^{(\alpha)} \) is the system Hamiltonian, see Methods for details. The phonon spectrum, unlike the eigenstates, does not change if \( \alpha = A \) is replaced with \( B \). Fig. 2a shows the phonon spectra of the soliton crystals with \( S_A = S_B \). The values of \( \beta_{k,n} \) scale with the linewidth, \( \kappa \), which, in the chip-integrated microresonators, varies in the range from tens to hundreds of MHz. The continuum of states starts around \( \beta_{k,n} \approx \pm \delta \) and is shaped like a typical band structure. Fig. 2b narrows the view to the top edge of the continuum, where one can see the band-crossing feature and bandgap (yellow shading). \( d_3 \neq 0 \) produces the small amplitude dispersive waves with the strongly tilted straight-line spectrum, see Fig. 2.

When \( S_A \) becomes \( \neq S_B \), either way, the band crossing opens up to the bandgap, see the blue shading in Fig. 2. At the same time, the yellow shaded \( S_A = S_B \) band gap starts narrowing and comes to the near band-crossings for \( S_{A,B} = \pi(1 \pm 0.5)/K \), see Fig. 2. We recall that the textbook SSH chain with the nearest-neighbour coupling has only two bands that cross at the Brillouin zone edges when the inter and intra-cell coupling rates \( (r \text{ and } r') \) are equal. The topological gap opens up for \( r \neq r' \), and its width equals \( |r - r'| \). Thus, the first two bands in the soliton crystal lattice behave very similarly to what happens in the SSH chain. To some extent, the similarity with the SSH model comes unexpectedly, since the spectrum of the Jacobian operator, \( \hat{\sigma}_z \hat{H}_k^{(\alpha)} - i\frac{1}{2} \kappa \mathbf{1} \), defines the phonon band structure in soliton crystals, while in the SSH model \([4]\), and for the non-interacting electrons in crystals \([44]\), this is the Hamiltonian spectrum.

**Geometrical phase and Wannier-centres**

If the soliton crystal is considered from the same point of view as the ionic crystal lattice shaping clouds of bound electrons in dielectrics, then the next natural step would be to understand the shapes of the phononic clouds existing around the solitons. This is achieved by devel-
The magenta ($\alpha = S$) point $\pi$ on crystals numerically by observing the eigenvalue solver. Applicable to any Bloch-function phases generated by the occurrences for every $k$-crystals, see Methods. The simultaneous bra and ket of phonons belonging to a specific band in the soliton (BZ) [44, 62–64]. The electron acquired after its passage over the Brillouin zone (Zak) phase of an electron, see Eq. [19]. The magenta ($\alpha = B$) and blue ($\alpha = A$) vertical dotted lines mark the values of $Z_n^{(\alpha)}/K$ from (a). (d) shows three selected profiles of $|V_{j,0}^{(\alpha)}|$ for $S_A$ marked by the white horizontal lines in (c).

FIG. 3. Geometrical (Zak) phases and Wannier functions in soliton metacrystals. (a,b) Numerically computed Zak phases for the $n = 0$ (a) and $n = 1$ (b) bands. The phases flip by $\pi$ at the band-crossing points, cf. Fig. [2]. (c) The change of the positions and relative strength of the peaks of the $n = 0$ Wannier function vs the soliton separation, $S_\alpha$, and $\theta - \theta_J$ (restricted to the one and a half unit cell length to boost resolution). The black-orange colour-map shows $|V_{j,0}^{(\alpha)}|$, see Eq. [19]. We check topological properties of phonons in soliton metacrystals. (a) Numerically computed Zak phases for the $n = 0$ (a) and $n = 1$ (b) bands. The phases flip by $\pi$ at the band-crossing points, cf. Fig. [2]. (c) The change of the positions and relative strength of the peaks of the $n = 0$ Wannier function vs the soliton separation, $S_\alpha$, and $\theta - \theta_J$ (restricted to the one and a half unit cell length to boost resolution). The black-orange colour-map shows $|V_{j,0}^{(\alpha)}|$, see Eq. [19]. The magenta ($\alpha = B$) and blue ($\alpha = A$) vertical dotted lines mark the values of $Z_n^{(\alpha)}/K$ from (a). (d) shows three selected profiles of $|V_{j,0}^{(\alpha)}|$ for $S_A$ marked by the white horizontal lines in (c).

The $k$-space periodicity and gauge-freedom properties of the Bloch vectors are,

$$u_{k,n}^{(\alpha)} = u_{k+K,n}^{(\alpha)} e^{iK\theta}, u_{k,n}^{(\alpha)} \rightarrow u_{k,n}^{(\alpha)} e^{i\xi_k}.$$  

Here, $\xi_k$ are the phases, which are arbitrary across the first BZ and extendable beyond it with $\xi_k = \xi_{k+K}$. The discreteness of $k$ requires special care when formulating the gauge invariant computational strategy for the geometric phase. Adopting the approach of [63] [64], we have derived the following equation for the geometric phase,

$$Z_n^{(\alpha)} = \text{Im} \ln \prod_{k=1}^K \langle u_{k,n}^{(\alpha)} | \hat{\sigma}_z | u_{k+1,n}^{(\alpha)} \rangle,$$  

of phonons belonging to a specific band in the soliton crystals, see Methods. The simultaneous bra and ket occurrences for every $k$ make Eq. [7] gauge invariant and applicable to any Bloch-function phases generated by the eigenvalue solver.

We check topological properties of phonons in soliton crystals numerically by observing the $\pi$-flipping of their geometric phase on dragging the system through the band crossing points. Figs. 3a,b show $Z_n^{(\alpha)}$ vs $S_\alpha$ for $n = 0,1$. The $n = 0$ phase flips from $-\pi$ to zero at the point $S_{A,B} = \pi/K$, where the $n = 0$ and $n = 1$ bands make the near-crossing, see Fig. [2]. The topology of the $n = 1$ band reflects on the co-existence of one crossing with the $n = 0$ band and two crossings with the $n = 2$ band, and, hence, its geometrical phase flips three times.

If the number of cells is taken to infinity while their length is kept fixed at $2\pi/K$, then $k$ becomes continuous and, hence, $\partial_k$ is well defined. In this limit, the geometric phase acquires a more familiar form, $Z_n^{(\alpha)} = \int K A_{k,n}^{(\alpha)} dk$, where $A_{k,n}^{(\alpha)} = i\langle u_{k,n}^{(\alpha)} | \hat{\sigma}_z \partial_k | u_{k,n}^{(\alpha)} \rangle$. $A_{k,n}^{(\alpha)}$ differs from the Berry connection for the non-interacting electrons [43] [44] by the Pauli matrix $\hat{\sigma}_z$ before $\partial_k$. Taking a unit cell with the coordinate $\theta = \theta_J$ and defining the corresponding Wannier function as $|w_{j,0}^{(\alpha)}| = K^{-1} \sum_k |u_{k,n}^{(\alpha)}| e^{ik(\theta - \theta_J)}$, we have further demonstrated that the geometric phase is directly proportional to the averaged coordinate of the phononic cloud centre in a given cell,

$$Z_n^{(\alpha)} = \langle w_{j,0}^{(\alpha)} | \hat{\sigma}_z (\theta - \theta_J) | w_{j,0}^{(\alpha)} \rangle.$$  

With $\hat{\sigma}_z \rightarrow \hat{1}$, the above would be the equation for the band- or Wannier-centre of the electron wave function in a crystal [44] [62] [63], see Methods for more details. For our unit cell definition, see Fig. [1] the $n = 0$ phonon Wannier centres can be located either in the middle or at the boundary of a unit cell. Figs. 3a–d are explicit about the matching between $Z_n^{(\alpha)}/K$ and the geometric centres of the Wannier functions. Recent papers demonstrating measurements of the geometric phases of cold atoms in optical lattices [65] and light in waveguide ar-
rays [66, 67] have applied various practical methods to detect positions of the respective wave-packets.

Metacrystals with defects: Edge states and chirality

For the SSH model, creating the lattice defect by removing one A-type unit cell, i.e., breaking two strong bonds in the chain, introduces the edge state inside the bandgap [4]. To study the bandgap states in the soliton metacrystals, we first extracted one pair of solitons and then tuned $S_{A,B}$, see Fig. 4. The corresponding phonon spectrum plotted as a function of $S_{A}$, see Fig. 4b, shows the near-crossing of the two bands at $S_{A} = \pi/K$, and the state inside the bandgap emerging for $S_{A}$ either $< \pi/K$ ($B$-type defect) or $> \pi/K$ ($A$-type defect). The eigenvectors of the bandgap state are localised around the defect on either side from $\pi/K$, see Fig. 4c. For $\alpha = A$, the state vector is localised on the edge solitons, while, for $\alpha = B$, it is guided in the middle of the defect, see Fig. 4c. The data presentation for the SSH edge states similar to the style chosen in Figs. 4b,c can be found in [49].

If the defect is made by the odd number of solitons, then shifting between the $\alpha = A$ and $\alpha = B$ dimerizations corresponds to moving the weak bond from one side of the defect to the other, see, e.g., the structure of the 7-soliton defect in Fig. 5a. Then, the edge state also migrates together with the weak bond, see Fig. 5b. With the defects larger than one unit cell, the spectrum in the bandgap contains not only the edge state but also other states guided inside the defect not at its edges, see the black dotted lines inside the blue shading in Fig. 5b. The guidance mechanism for these modes is akin to the band-gap guidance in the hollow-core photonic crystal fibres [68].

The defects consisting of the odd-number of solitons break the left-right symmetry of the metacrystals and thereby appear as an interesting object to study the spatio-temporal and spectral manifestations of chirality [55]. We consider a crystal to be chiral, providing that the mirror image of the solitons around the defects can not be made to coincide with the original soliton arrangement. This is true for any $S_{A} \neq S_{B}$, while, the $S_{A} = S_{B} = \pi/K$ case corresponds to the achiral defect. Indeed, the unpaired soliton can be removed either on the left or right side of the defect, and then the two crystals with the same $S_{A}$ are connected by the chiral symmetry transformation. Tuning $S_{A}$ and plotting the crystals around the defect edges makes the chirality obvious, see the tilts of the solitons at the defect edges in Figs. 5a and 5b.

The chiral pairs of the right and left defects have the spectra which are hard to distinguish. Therefore, we have just shown one of them in Fig. 5a. The spectrum of the achiral defect is shown for comparison in Fig. 5b. The envelope of the large amplitude spectral lines match well with the spectra of the ideal crystals, while the small amplitude dense spectrum originates from the defect. To make the spectral signature of the chirality effect obvious, we have taken the frequency spectra of the left and right defects, i.e., $\hat{\omega}_{\mu}^{(left)}$ and $\hat{\omega}_{\mu}^{(right)}$, and subtracted from them the achiral spectrum, $\hat{\omega}_{\mu}^{(ac)}$. Here, $\hat{\omega}_{\mu} = \omega_{\mu} + \mu \hat{D}_{\mu}^{(-)}$ is
FIG. 5. Chirality of soliton metacrystals with defects. (a,b) show metacrystals with the differently arranged 7-soliton defects and $K = 24$. (a) and (b) geometries are called left and right, respectively. The missing soliton locations are marked with dashed lines. Note that the $\theta$-interval shown is $< 2\pi$. (c,d) show the examples of spectra of the achiral and chiral defects. (e) shows the normalised frequency spectra of the crystals with the right and left defects, i.e., $\tilde{\omega}_\mu^{(\text{right})}$ and $\tilde{\omega}_\mu^{(\text{left})}$, minus the $\tilde{\omega}_\mu^{(\text{ac})}$ spectrum corresponding to the achiral geometry, $S_\alpha = \pi/K$. Red dots correspond to the right defect, $(\tilde{\omega}_\mu^{(\text{right})} - \tilde{\omega}_\mu^{(\text{ac})})/\kappa$, and blue dots to the left one, $(\tilde{\omega}_\mu^{(\text{left})} - \tilde{\omega}_\mu^{(\text{ac})})/\kappa$. The values of $\mu$ shown are restricted to $\mu \in [360, 1200]$, with the step being 120.

Discussion

We have conjectured and confirmed numerically that the train of solitons in microresonators can be considered as a spatio-temporal topological metamaterial, i.e., soliton metacrystals. The optical spectra of such crystals correspond to the octave wide frequency combs. The elementary excitations, i.e., phonons, in metacrystals are the radio to terahertz modulations propagating across the spectrum of the resonator modes. We have computed the phononic Bloch states and their geometrical (Zak) phases. The Zak phase has also been expressed via the Wannier functions and demonstrated to have the meaning of the effective polarization of the phononic clouds around the solitons.

Zak phase changes in the steps of $\pi$ with the tuning of the soliton separation, which proves the non-trivial topology of the metacrystal band structure. Further to this point, we have found the phononic edge states upon introducing the one unit cell and larger defects. We have demonstrated that the optical (photon) spectra of metacrystals with the left and right defects can be used to characterize chirality in time. Subtracting the optical spectrum of the achiral crystal from the chiral ones reveals the butterfly structure of frequencies, see Fig. 5e, similar to the butterfly wings illustrating chirality in nature.

Features of the proposed realisation of the SSH-like soliton lattice are in its spatio-temporal and dissipative nature and that it does not require spatial or temporal modulations of the material refractive index and pump laser and fabrication of the complex arrays of coupled resonators and waveguides. Further, we should note that one out of twenty microresonator soliton crystals illustrated in [14] shows the SSH-like arrangement of soliton molecules with several embedded defects, see Fig. 3j. This suggests that the frequency combs with topological properties may have already been unintentionally captured in the experimental measurements. Our results intend to motivate further theory, experiments and applications so that this topic can grow and take its place in the interdisciplinary areas of topological and ultrafast physics. We are also forecasting applications of the soliton metacrystals and their topological states in classical and quantum information processing, where the microresonator solitons and topological photonics are already making an impressive start [69–73].

METHODS

In order to shorten notations we have dropped the band index, $n$, and the dimerization superscript, $(\alpha)$, in the
first part of Methods. They are subsequently reintroduced in the second and third parts.

**Bloch formalism**

To analyse and solve Eq. (1) we set the ansatz consisting of the time independent solution which could be a crystal with or without defect, \( \Phi(\theta) = \Phi(\theta + 2\pi) \), plus the small amplitude phonon field, \( \tilde{\phi}(\theta, t) \). Hence,

\[
\phi = \Phi(\theta) + \tilde{\phi}(\theta, t), \quad \tilde{\phi}(\theta, t) = \tilde{\phi}(\theta + 2\pi, t).
\]  

(1.1)

Linearising Eq. (1) for \( \tilde{\phi} \) yields

\[
i(\partial_t + \frac{1}{2}\kappa) \left( \frac{\partial}{\partial \theta} \right) \tilde{\phi} = \tilde{\sigma}_z \tilde{H}_0 \left[ \frac{\partial}{\partial \theta} \right] \tilde{\phi}, \quad \theta \in [0, 2\pi),
\]

(1.2)

where \( \tilde{H}_0 \) is specified in Eq. (m.8).

We now assume that \( \Phi(\theta) \) has a period \( 2\pi/K \), where \( K \) could also be one,

\[
\Phi(\theta) = \sum_k \phi_k e^{iK\theta} = \Phi \left( \theta + \frac{2\pi}{K} \right).
\]

(1.3)

Equations for \( \phi_k \) are obtained using the Newton method. Parameters used are typical for Si\(_3\)N\(_4\) resonators: \( D_1/2\pi = 100\)GHz, \( D_2/2\pi = 50\)kHz, \( D_3/2\pi = 50\)Hz, \( \gamma/2\pi = 300\)MHz/W, \( k/2\pi = 100\)MHz and laser power \( W = 520\)mW, so that \( \hbar^2 = (D_1/2\pi\kappa)W = 83\)W, see Eqs. (1)-(3) and Ref. [56] for further parameter and model discussion. The scaled values of the parameters are given in the Fig.1 caption. The approximate analytical expressions for the non-topological soliton crystals in the Lugliato-Lefever equation have been reported in, e.g., [74, 75].

The phonon field is set as [76, 77]

\[
\tilde{\phi} = \sum_{k=1}^{K} \left[ x_k(t, \theta)e^{ik\theta} + y_k(t, \theta)e^{-ik\theta} \right],
\]

(1.4)

\[
x_k = X_k(\theta)e^{-i\beta_k t + i\lambda_k}, \quad y_k = Y_k(\theta)e^{-i\beta_k t - i\lambda_k}.
\]

(1.5)

Here, \( k \) is the Bloch angular momentum. \( X_k(\theta) \) and \( Y_k(\theta) \) are the cell-periodic functions, i.e., have the same periodicity as \( \Phi(\theta) \), therefore their Fourier series are

\[
X_k(\theta) = \sum_l X_{k,l}e^{iK\theta}, \quad Y_k(\theta) = \sum_l Y_{k,l}e^{iK\theta}.
\]

(1.6)

Substituting Eq. (1.4) into Eq. (1.2) gives

\[
i(\partial_t + \frac{1}{2}\kappa) \langle Q_k \rangle = \tilde{\sigma}_z \tilde{H}_k \langle Q_k \rangle, \quad \langle Q_k \rangle = \frac{x_k}{|y_k|},
\]

(1.7)

\[
\tilde{H}_k = \begin{bmatrix} \tilde{D}_k & -\gamma \Phi^2 \\ -\gamma \Phi^2 & \tilde{D}_k \end{bmatrix}, \quad \theta \in [0, 2\pi/K),
\]

(1.8)

\[
\tilde{D}_k = \delta - 2\gamma|\Phi|^2 + \sum_{l \geq 1} \frac{d_{lK}}{l^2} (k - il\theta)^2,
\]

(1.9)

and then, applying Eq. (1.3), we find

\[
(\beta_k + i\lambda_k + \frac{1}{2}\kappa) |u_k\rangle = \tilde{\sigma}_z \tilde{H}_k |u_k\rangle, \quad |u_k\rangle = \begin{bmatrix} X_k \\ Y_k \end{bmatrix}.
\]

(1.10)

The above is Eq. (5) in the main text. One computational advantage of the Bloch formalism comes from the property that

\[
\beta_k = \beta_{k+K}, \quad \lambda_k = \lambda_{k+K}, \quad |u_k\rangle = |u_{k+K}\rangle e^{iK\theta},
\]

(1.11)

and, therefore, \( k \) can be restricted to a single Brillouin zone, \( k = 1, 2, \ldots, K \). The other is that the spectral bandwidth \( \mu \in [-\mu_{\text{max}}, \mu_{\text{max}}] \), see Eq. (1), is now achieved by taking \( l \in [-l_{\text{max}}, l_{\text{max}}] \), with \( l_{\text{max}} = \mu_{\text{max}}/K \).

For \( K \) starting from 2 and above, this allows to work with the proportionally smaller number of modes when Eq. (m.9) is solved in the Fourier space.

**Geometrical phase and gauge invariance**

The Zak phase formalism that needs to be developed for the soliton metacrystals should reflect on two features - (A) nonlinear interaction between the phonon and crystal and (B) the discrete sampling of the states in the Brillouin zone. In order to make our derivations transparent, we first neglect (B) and, hence, take the limit of a large number of unit cells, so that \( k \) is continuous in the Brillouin zone. \( k \) is now assumed to vary adiabatically in time, \( k = k(t) \). The equation of motion, Eq. (m.7), for the phonon wave function, \( |Q_{k,n}^{(\alpha)}\rangle \), is solved by the substitution [43, 44]

\[
|Q_{k,n}^{(\alpha)}\rangle = f_{k,n}(t) |u_{k,n}^{(\alpha)}\rangle,
\]

(1.12)

where \( f_{k,n}^{(\alpha)} \) is the function to be found and the phonons are assumed confined to the band \( n \). For \( |\omega_{k,n}| \gg |\lambda_{k,n}|, \kappa \), the left eigenvector of \( \tilde{\sigma}_z H_k^{(\alpha)} \) is \( |u_{k,n}^{(\alpha)}\rangle |\tilde{\sigma}_z |76\rangle \). Substituting Eq. (1.11) to Eq. (m.8) and projecting leads to

\[
i \frac{d f_{k,n}^{(\alpha)}}{dt} \approx \beta_{k,n} \partial_t - A_{k,n}^{(\alpha)} dk,
\]

(1.13)

\[
A_{k,n}^{(\alpha)} = \frac{i}{N_n} \langle u_{k,n}^{(\alpha)} | \tilde{\sigma}_z \partial_k | u_{k,n}^{(\alpha)} \rangle, \quad N_n = \langle u_{k,n}^{(\alpha)} | \tilde{\sigma}_z | u_{k,n}^{(\alpha)} \rangle,
\]

(1.14)

where \( N_n \) is the normalization constant.

The \( \beta_{k,n} \) and \( A_{k,n}^{(\alpha)} \) terms in Eq. (1.12) are the instantaneous dynamical and geometrical phases. Hence, the total geometric phase acquired during \( k(t) \) passing the first Brillouin zone (BZ) is

\[
Z_n^{(\alpha)} = \int_{\text{BZ}} A_{k,n}^{(\alpha)} dk.
\]

(1.15)

Our \( A_{k,n}^{(\alpha)} \) differs from the Berry connection emerging in the linear problems [11, 43, 44], by the Pauli matrix \( \tilde{\sigma}_z \), before \( \partial_k \), which has been previously reported in, e.g., photonic crystals with parametric gain [55] and LC-circuits [43, 44]. The normalisation condition applied by us is \( N_n = \pm 1 \), see, e.g., [58, 76] for how similar norms appear in the theory of Bose condensates. \( \tilde{\sigma}_z \) also enters the Berry curvature of the Bogolyubov excitations of Bose condensates [78].
The phases of the Bloch functions are not uniquely defined and can be changed by the gauge transform, which, in the discrete BZ, takes the form

\[ u_{k,n}^{(a)} \rightarrow u_{k,n}^{(a)} e^{i\xi_k}, \quad \xi_k = \xi_{k+K}. \] (m.14)

For the k-continuous, \( Z_n^{(a)} \) remains invariant on applying Eq. (m.14) \[ \text{[14]} \]. When \( k \) is sampled discretely, a variety of available numerical schemes to deal with \( \delta_k \) will not generally comply with the gauge invariance. Therefore, designing a practical algorithm to compute \( Z_n^{(a)} \) is an important issue to consider.

This brings us to the point (B) and we assume that \( k \) is advancing in the unitary steps from 1 to \( K \), and each step takes the time \( dt \) to make, then Eq. (m.12) updates as

\[ i \left( f_{k+1,n}^{(a)} - f_{k,n}^{(a)} \right) \approx \beta_{k,n} dt \] (m.15)

\[ -i \left( \langle u_{k,n}^{(a)} | \hat{\sigma}_z | u_{k+1,n}^{(a)} \rangle - \langle u_{k,n}^{(a)} | \hat{\sigma}_z | u_{k,n}^{(a)} \rangle \right) / N_n, \]

and, therefore, the total geometric phase is

\[ Z_n^{(a)} = -i \sum_{k=1}^{K} \left( \langle u_{k,n}^{(a)} | \hat{\sigma}_z | u_{k+1,n}^{(a)} \rangle - N_n \right) / N_n. \] (m.16)

Checking of Eq. (m.16) reveals the discretization scheme induced violation of the gauge invariance. Indeed, Eq. (m.16) is invariant on applying \( (u_{k,n}^{(a)}, u_{k+1,n}^{(a)}) \) \( \rightarrow \) \( (u_{k,n}^{(a)} e^{i\xi_k}, u_{k+1,n}^{(a)} e^{i\xi_k}) \) and not relative to Eq. (m.14).

The recipe to restore the gauge invariance is given by the theory of polarization in crystalline solids \[ \text{[63, 64]} \]. We first take the exponent from Eq. (m.16), and then use \( e^{z} = 1 + x + \ldots \),

\[ \exp \left\{ i Z_n^{(a)} \right\} = \prod_{k=1}^{K} \exp \left\{ \langle u_{k,n}^{(a)} | \hat{\sigma}_z | u_{k+1,n}^{(a)} \rangle \frac{1}{N_n} - 1 \right\} \]

\[ \approx \prod_{k=1}^{K} \langle u_{k,n}^{(a)} | \hat{\sigma}_z | u_{k+1,n}^{(a)} \rangle \frac{1}{N_n}. \] (m.17)

Taking the logarithm gives the gauge invariant expression for the geometric phase of the soliton crystals,

\[ Z_n^{(a)} = \text{Im} \ln \prod_{k=1}^{K} \langle u_{k,n}^{(a)} | \hat{\sigma}_z | u_{k+1,n}^{(a)} \rangle \frac{1}{N_n} \] (m.18)

\[ = \text{Im} \ln \left\{ \frac{1}{N_n^K} \times \langle u_{2,n}^{(a)} | \hat{\sigma}_z | u_{2,n}^{(a)} \rangle \langle u_{3,n}^{(a)} | \hat{\sigma}_z | u_{3,n}^{(a)} \rangle \ldots \langle u_{K,n}^{(a)} | \hat{\sigma}_z | u_{K,n}^{(a)} \rangle \langle u_{1,n}^{(a)} | \hat{\sigma}_z | u_{1,n}^{(a)} e^{-iK\theta} \rangle \right\}. \]

\'Im' is defined by its principal value, such that \( Z_n^{(a)} \) \( \in \) \([-2\pi, 0)\). For \( K \) even, \( N_n^K = 1 \) and the above coincides with Eq. (7) in the main text.

Wannier formalism

The direct and inverse Bloch-to-Wannier transforms are defined as

\[ |u_{k,n}^{(a)}\rangle = \sum_{J} |w_{J,n}^{(a)}\rangle e^{-ik(\theta_{J}-\theta)} = \left[ \begin{array}{c} X_{k,n}^{(a)} \\ Y_{k,n}^{(a)} \end{array} \right], \]

\[ |w_{J,n}^{(a)}\rangle = \frac{1}{K} \sum_{k} |u_{k,n}^{(a)}\rangle e^{ik(\theta_{J}-\theta)} = \left[ \begin{array}{c} W_{J,n}^{(a)} \\ V_{J,n}^{(a)} \end{array} \right], \] (m.19)

where \( |w_{J,n}^{(a)}\rangle \) are Wannier functions, \( \theta_{J} = 2\pi(J-1)/K \) and \( J \in \mathbb{Z} \) numbers the unit cells. Our gauge choice for the Bloch functions is specified by the condition \( \text{Im} X_{k,n}^{(a)} = 0 \) at the point \( \theta = 3\pi/2K \).

We now recall Eq. \( \text{[m.9]} \) and, then, transform Eq. \( \text{[m.13]} \),

\[ \mathcal{Z}^{(a)} = i \int_{BZ} dk \langle u_{k,n}^{(a)} | \hat{\sigma}_z \partial_k | u_{k,n}^{(a)} \rangle \] (m.20)

\[ = i \int_{BZ} dk \int_{\theta_J - \pi/K}^{\theta_J + \pi/K} \left( X_{k,n}^{(a)} \partial_k X_{k,n}^{(a)} - Y_{k,n}^{(a)} \partial_k Y_{k,n}^{(a)} \right) d\theta \]

\[ = \frac{i}{K} \int_{BZ} \int_{\theta_J - \pi/K}^{\theta_J + \pi/K} \left( X_{k,n}^{(a)} \partial_k X_{k,n}^{(a)} - Y_{k,n}^{(a)} \partial_k Y_{k,n}^{(a)} \right) d\theta. \]

The last part of Eq. (m.20) uses the fact that the Bloch functions are cell periodic and, hence, the integration can be extended to the entire ring.

If the ring is large, the problem can be well approximated by the straight-line infinite crystal lattice \[ \text{[44]} \] with the period \( 2\pi/K \). Then, \( \sum_{k} \rightarrow \int_{BZ} dk \) and expressing the Bloch functions via the Wannier ones allows to take the \( k \)-derivative inside Eq. (m.20),

\[ \mathcal{Z}^{(a)} = \sum_{J} \int_{\theta_J - \pi}^{\theta_J + \pi} \left[ |W_{J,n}^{(a)}|^2 - |V_{J,n}^{(a)}|^2 \right] (\theta - \theta_J) d\theta \]

\[ = \sum_{J} \langle w_{J,n}^{(a)} | \hat{\sigma}_z (\theta - \theta_J) | w_{J,n}^{(a)} \rangle. \] (m.21)

Wannier functions for all \( J \) coincide if plotted vs \( \theta - \theta_J \), therefore, Eq. (m.21) simplifies to

\[ \mathcal{Z}^{(a)} = K \langle w_{J,n}^{(a)} | \hat{\sigma}_z (\theta - \theta_J) | w_{J,n}^{(a)} \rangle, \] (m.22)

see Eq. (8) in the main text. Thus, the geometric phase of soliton crystals is determined by the coordinate of the effective centre of the phonon cloud in the unit cell, i.e., by the Wannier-centre, \( \langle w_{J,n}^{(a)} | \hat{\sigma}_z (\theta - \theta_J) | w_{J,n}^{(a)} \rangle \). For the ring geometry with the relatively large number of unit cells, as we are dealing with, Eq. (m.22) remains a good approximation.

Data availability

The data supporting the findings of this study are available from authors on reasonable request.

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