

Metastability, chaos, and spectrum tomography for Bose-Hubbard rings and chains

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We analyze the metastability of Bose-Hubbard condensates for finite-size one-dimensional ring lattices and open chains, using a semiclassical tomographic perspective that emphasizes the relation of the many-body spectrum to the underlying classical phase-space structures. In order to address quantum ergodicity in far-from-equilibrium scenarios of experimental interest, we inspect both local aspects (via Bogoliubov analysis) and global aspects (mixed regular-chaotic dynamics). In particular, we highlight the roles of the two parameters that control metastability, clarify the essential differences between low- and high-dimensional chaos, and show how the dynamical instabilities diminish in the limit of the Gross-Pitaevskii equation. It is somewhat frustrating that with more degrees of freedom, the dynamically metastable islands become better distinct from the ergodic sea, while their borders become ill-defined topologically. This stands in opposition to the very structured phase space of two-degree-of-freedom systems, as reflected in the tomographic quantum spectrum.

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I. INTRODUCTION

Condensation is a central theme in the theory of superfluidity (SF), and in some sense also in the theory of superconductivity [1–3]. The essence of SF is the feasibility of observing a metastable persistent current. An appropriate geometry for demonstrating SF is an L_s -site ring with bosons. The standard version is described by the Bose-Hubbard Hamiltonian (BHH) [4,5], which generates the dynamics of N bosons, with intersite hopping K and on-site repulsive interaction U . The two-site version, also known as bosonic Josephson junction, is well studied [6–9]. The minimal version for a ring requires $L_s = 3$ sites, also known as trimer [10–22].

The *classical* equations of motion for an L_s -site ring or chain, which are generated by the BHH, are known as the discrete nonlinear Schrödinger equation (DNLSE) [23,24]. In the continuum limit, one obtains the Gross-Pitaevskii equation (GPE). From a classical perspective, the dimer is integrable, while the trimer features a phase space with a mix of quasiregular and chaotic dynamics. Its analysis provides many insights regarding the feasibility of observing a metastable condensate [25–27]. However, the trimer is non-generic in many respects, as clarified below. Our purpose is to extend the perspective. In particular, we would like to place the emphasis on the questionable metastability of condensates in Bose-Hubbard chains with $L_s > 3$ sites. We also intend to clarify the GPE limit ($L_s \rightarrow \infty$) where chaos is diminished, and integrability is recovered.

The BHH has inspired an extensive experimental work. The formation of lattices for trapping Bosons is state of the art (see Ref. [28] and references therein). The bosons can be trapped by a painted optical potential (see, e.g., Fig. 11 there). Optionally, the ring can be rotated (control over the scaled rotation velocity Φ , also known as Sagnac phase). The occupation of the momentum orbitals or the current can be measured from time-of-flight images (see, e.g., Fig. 15 there). See, for example, experiments reported in Refs. [29,30]. The questions that we ask regarding metastability concern far-from-equilibrium scenarios of experimental interest, in particular, in box geometry [31–36] or possibly after invoking turbulence [37–41].

Phase space. Formally, the BHH describes coupled nonlinear oscillators and therefore provides an ideal arena for the study of “quantum chaos” themes [26,42–49]. Taking into account that N is a constant of motion, the BHH has effectively $d = L_s - 1$ degrees of freedom (dof). For $L_s = 2$, the phase space is the Bloch sphere, while for $L_s = 3$ it is a four-dimensional (4D) space. In the latter case, the energy surface is three dimensional (3D), whereas the Kolmogorov-Arnold-Moser (KAM) tori are two-dimensional surfaces [50]. It follows that chaotic regions are strictly separated by the KAM tori. If L_s is larger, the d -dimensional KAM tori cannot divide the $2d - 1$ energy surface into distinct regions: Even if the nonlinearity is small, we have in principle Arnold diffusion [51,52]. Thus, $L_s = 3$ is, in fact, nongeneric. Generic chaos requires $L_s > 3$.

Ground state. Semiclassically, the ground state of the BHH can be visualized as a squeezed Gaussian located at the minimum of the energy landscape. Formally, the minimum is a stationary point (SP) of the Hamiltonian flow. If U is large (compared to N^2), the squeezed Gaussian cannot be accommodated within the island that surrounds this SP, leading to a transition to a Mott insulator (MI) state.

Energetic metastability. The L_s -site BHH has L_s single-particle orbitals. Each orbital is formally a trivial SP in phase

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space. For example, for $L_s = 2$, these orbitals are the west and east poles of the Bloch sphere (the north and south poles correspond to the two sites of the system). If the SP is a local minimum, its island possibly can accommodate a squeezed Gaussian, and then we say that we get an energetically stable (ES) condensate. This is the type of stability that has been discussed by Landau (the “Landau criterion”), i.e., thermodynamically stable SP. As pointed out by Leggett [1], this type of metastability is feasible for condensate in a ring, but *not* for a condensate in a box. We shall inquire further this observation in the present work.

Dynamical metastability. If the SP is neither a local minimum nor a local maximum, then it is a saddle point of the energy landscape. There is a simple way to diagnose such a case: The Bogoliubov frequencies of the SP do not have the same sign or become complex. The latter option implies that the SP is dynamically unstable, whereas the former option opens the possibility to observe dynamical stability (DS).

Quantum DS. The question arises whether a dynamically stable SP can support a metastable condensate. The reasoning is based on the idea that the SP should be surrounded by a large enough stability island that can accommodate a squeezed Gaussian. The role of the Planck constant is played here by $1/N$. Then, the feasibility of a DS condensate is based on the prevailing semiclassical eigenfunction hypothesis of Percival [53,54], who suggested a classification of quantum mechanical spectra into “regular” and “irregular” eigenstates, supported, respectively, by quasiregular islands and chaotic seas. This conjecture, that eigenstates can be associated with phase-space regions, is complementary to Berry’s conjecture [54,55], and to the eigenstate thermalization hypothesis [56–64].

Quantum hybrids. In practice, it is likely to observe hybrid eigenstates that do not respect Percival’s conjecture. Rather, they form a superposition of pieces that are localized in different regions in phase space. This has been demonstrated in Ref. [65]. It possibly can be regarded as a variant of chaos-assisted tunneling [66], or as amphibious eigenstates that ignore the classical structures [67].

Quantum scarring. Even if we do not have a stability island, there might be a possibility for the SP to support a condensate. In particular, it has been demonstrated [65] that an unstable SP of an $L_s = 3$ chain can localize a wave packet and, hence, support a metastable condensate. But the latter option is rather exotic, and fragile, and better be regarded as a “quantum scarring” effect [68–72].

Tomography. Rather than asking yes/no questions about metastability versus ergodization, we prefer to use the traditional “quantum chaos” perspective, namely, we look for the quantum *signatures* of ES/DS and chaos. The common practice is to look on the energy level statistics. But such an approach has two issues: (1) It provides numerically clear results only for rather simple systems with large N , such that the spectrum in the range of interest is dense enough, and (2) it does not allow classification of the eigenstates in the typical situation of underlying mixed chaotic and quasiregular dynamics. As opposed to that, our approach [73] is *numerically cheap* and flexible enough to deal with small complex systems. We use the term *quantum phase-space tomography* in order to emphasize that the inspection of the spectrum is not

limited to “level statistics,” but rather oriented to reveal the detailed relation to the underlying phase-space structures that serve as a classical skeleton for the quantum eigenstates. A useful practice is to provide 3D images of the spectrum. Each point in such an image represents an eigenstate, whose vertical position is the energy. The extra dimensions (horizontal axis/axes and/or color code) are exploited to reveal properties of the eigenstates. Such a technique has been exploited, e.g., to highlight Monodromy-related features in the spectrum [74].

Outline. We introduce the model, its semiclassical limit, and its continuum GPE limit in Secs. II, III, and IV, respectively. The energy landscape discussed in Sec. V motivates the Bogoliubov stability analysis presented in Secs. VI–VIII, leading to the big picture of stability regimes in Sec. IX. After inspection of representative trajectories in Sec. X, we present both quantum and classical tomography of the spectrum in Sec. XI. Furthermore, we show in Sec. XII how the transitions between the stability regimes are reflected. Quantum ergodicity is then carefully inspected in Sec. XIII. We conclude our findings in Sec. XIV.

II. MODEL HAMILTONIAN

Consider a system with L_s equally spaced sites x_j , labeled by j . The BHH is expressed in terms of Fock operators $\mathbf{a}_j$ and associated site occupation operators $\mathbf{n}_j = \mathbf{a}_j^\dagger \mathbf{a}_j$. Given on-site potential V_j , intersite hopping K_{ji} , and on-site interaction U , it takes the form

$$\mathcal{H} = \sum_{j=1}^{L_s} \left[V_j \mathbf{a}_j^\dagger \mathbf{a}_j + \frac{U}{2} \mathbf{a}_j^\dagger \mathbf{a}_j^\dagger \mathbf{a}_j \mathbf{a}_j \right] - \sum_{\langle ij \rangle} \frac{K_{ji}}{2} \mathbf{a}_j^\dagger \mathbf{a}_i. \quad (1)$$

We assume below that the on-site potential is zero. For a chain, the nonzero couplings are $K_{j+1,j} = K_{j,j+1} = K$, where $1 \leq j < L_s$. For a ring, periodic boundary conditions are imposed, such that the nonzero couplings are $K_{j+1,j} = K \exp(i\Phi/L_s)$, and their conjugates, where j is defined mod(L_s). In the latter case, the Sagnac phase Φ is proportional to the rotation frequency of the device, and can be regarded as a control parameter, as in recent experiments [29,30]. The number of particles N is a constant of motion that plays the role of inverse Planck constant.

A. Phase space

We can define optional creation operators via a unitary transformation as follows: $\mathbf{a}_\alpha^\dagger = \sum_j \langle x_j | \alpha \rangle \mathbf{a}_j^\dagger$. The associated single-particle states, also known as orbitals, are $|\alpha\rangle = \mathbf{a}_\alpha^\dagger |\text{vacuum}\rangle$. We can regard each orbital as a point in phase space. For example, for two sites the $\{\alpha\}$ phase space is the two-dimensional Bloch sphere. Condensation of N particles in the α orbital means $[\mathbf{a}_\alpha^\dagger]^N |\text{vacuum}\rangle$. The α condensates can be regarded as a set of coherent states in the sense of Perelomov and Gilmore [75,76].

B. The k orbitals

The stationary single-particle states of the Hamiltonian are the k orbitals that are labeled by k . For a ring, these are the momentum orbitals with $k = k_m = [2\pi/L]m$, where m is an integer mod(L) and $L = L_s$ is the length of the ring. For a box,

the labeling is

$$k = k_m[\text{box}] = \frac{\pi}{L}m, \quad \text{with } m = 1, 2, \dots, \quad (2)$$

where $L = L_s + 1$.

Here, L rather than L_s should be regarded as the length of the box. The associated Fock occupation operators are labeled as $\mathbf{n}_k$, with subscript k instead of site-index j . The respective unperturbed ($u = 0$) Fock-basis states are indexed by $\{n_k\}$. For the associated Fock creation operators, we used the dedicated notation

$$b_k^\dagger = \sum_j \langle x_j | k \rangle a_j^\dagger. \quad (3)$$

For a ring, the coefficients are $\sqrt{1/L}e^{ikx_j}$, while for a chain they are $\sqrt{2/L} \sin kx_j$.

C. Eigenstates

After diagonalization of the Hamiltonian for N particles, we get the many-body eigenstates $|E_v\rangle$ that are indexed by v . The ring Hamiltonian has translational symmetry; hence, it decomposes into L blocks that differ by the total momentum $P \bmod(2\pi)$. For the sake of numerical efficiency, we consider only the $P = 0$ block. Likewise, in the case of the chain, we have mirror symmetry, and therefore, for the sake of numerical efficiency, we exclude the odd-parity states.

From each eigenstate, we can extract an associated distribution in $\{n_k\}$ space. In particular, we shall focus our attention on a selected orbital k_o , and will use the notation $P^v(n_o)$ for the associated probability distribution of its occupation and $\langle n_o \rangle$ for the respective expectation value. Furthermore, for a given eigenstate, we calculate the one-body reduced probability matrix

$$\rho_{ij}^{(v)} = \frac{1}{N} \langle a_i^\dagger a_j \rangle_v. \quad (4)$$

The (basis independent) purity of the state is

$$\mathcal{S} = \text{Tr}(\rho^2). \quad (5)$$

The inverse purity $1/\mathcal{S}$ reflects the number of participating orbitals. In particular, $\mathcal{S} = 1$ implies that all the particles are condensed in a single orbital. A major objective is to identify the conditions for the appearance of such states, to characterize their stability, and to identify the associated excitations.

III. SEMICLASSICAL LIMIT

Formally, the BHH describes coupled nonlinear oscillators, and therefore provides an ideal arena for the study of “quantum chaos” themes [26,42]. In a semiclassical context, one defines action-angle coordinates via

$$\mathbf{a}_j = \sqrt{\mathbf{n}_j} e^{i\varphi_j}, \quad (6)$$

and the Hamiltonian expressed as $\mathcal{H} = H(\boldsymbol{\varphi}, \mathbf{n})$ becomes similar (but not identical) to that of a superconducting Josephson circuit.

In a classical context, we regard the $\mathbf{a}_j$ as phase-space coordinates of “oscillators,” with $\bar{\mathbf{a}}_j$ interpreted as the conjugate coordinates. The classical equation of motion for $(d/dt)\mathbf{a}_j$ is the DNLSE. For the generated trajectory, we can calculate

$\langle \bar{\mathbf{a}}_j \mathbf{a}_j \rangle$ as a temporal average, and hence calculate the associated classical purity $\mathcal{S}$.

In the absence of interaction, condensation in the k_o orbital ($n_k = N\delta_{k,k_o}$) is a stationary state. We already pointed out that such condensate can be regarded as a coherent state in the sense of Perelomov and Gilmore [75,76]. In the Wigner-function picture, it is represented in phase space by a minimal Gaussian-like distribution of uncertainty width $2/N$ in n_o . With interaction, assuming that the condensate is *stable* (in the ES or in the DS sense), we expect to find an eigenstate with $\mathcal{S} \sim 1$, reflecting occupation $n_o \sim N$. Such an eigenstate possibly can be described as a *squeezed* coherent state. For very large interaction u , such states get fragmented, as discussed in detail in Ref. [73]. The discussion of this SF-MI transition is outside the scope of the present work.

IV. GPE LIMIT

The single-particle energies and the associated velocities in a tight-binding chain that has lattice constant ℓ are $\varepsilon_k = -K \cos(\ell k)$ and $v_k = K\ell \sin(\ell k)$. In the continuum limit, $v_k = (1/M)k$ with mass $M = (K\ell^2)^{-1}$. The dimensionless semiclassical interaction parameter of the BHH, which controls the local nonlinearity and the manifestation of chaos, is

$$u = \frac{NU}{K} = \ell NMg, \quad (7)$$

where $g = U\ell$. In the continuum limit, the DNLSE becomes the GPE with interaction g . The only dimensionless parameter that survives in the GPE limit is

$$u_L = Lu = L \frac{NU}{K} = \mathcal{L} NMg \equiv \frac{1}{2} \left(\frac{\mathcal{L}}{\xi} \right)^2, \quad (8)$$

where $\mathcal{L} = L\ell$, while ξ is known as the healing length. Fixing u_L , the parameter $u = u_L/L$ that controls the local chaos diminishes in the GPE limit (no chaos). In the numerics, we treat the GPE and the DNLSE on equal footing. The units of length are chosen such that the lattice constant is $\ell = 1$, and the units of time are chosen such that $K = 1$.

A particle that is placed in the orbital k_o has in the GPE limit kinetic energy $\mathcal{E} = (K/2)(([2]\pi/L)m_o)^2$. Condensing N particles in the same orbital implies that there is a shift in the potential floor, which is characterized by the parameter

$$\Delta = \frac{N}{\mathcal{L}}g = \frac{NU}{L}. \quad (9)$$

Accordingly, we identify two dimensionless parameters that are going to play an important role in the stability analysis of such condensate:

$$\text{GPE parameter} = \frac{\Delta}{\mathcal{E}} \sim \frac{u_L}{\pi^2 m_o^2}, \quad (10)$$

$$\text{DNLSE parameter} = \frac{\Delta}{K} = \frac{u_L}{L^2}. \quad (11)$$

The DNLSE parameter reflects the existence of the lattice. In other words, the DNLSE, unlike the GPE, features a finite bandwidth because the kinetic energy is bounded $\mathcal{E} = K[1 - \cos(k)]$. Once the DNLSE parameter becomes

less than unity, it is implied that the healing length ξ becomes smaller than the lattice constant ℓ , and hence outside of the GPE regime.

V. THE ENERGY LANDSCAPE

The standard textbook procedure is to transform the BHH to the momentum basis using Eq. (3). Here, we treat the chain and the ring on equal footing and transform the finite-size BHH to the appropriate orbital basis. The Hamiltonian takes the form

$$\begin{aligned}\mathcal{H} &= \sum_k \varepsilon_k \mathbf{b}_k^\dagger \mathbf{b}_k + \frac{U}{2L} \sum C[k] \mathbf{b}_{k'''}^\dagger \mathbf{b}_{k''}^\dagger \mathbf{b}_{k'} \mathbf{b}_k \\ &= \sum_k \varepsilon_k \mathbf{n}_k + \frac{U}{L} N^2 - \left[\frac{1}{2} \right]_c \frac{U}{2L} \sum_k \mathbf{n}_k^2 + \text{transitions},\end{aligned}\quad (12)$$

$$(13)$$

where $C[k] \equiv C[k''', k'', k']$ are combinatorial coefficients and $[1/2]_c$ is an extra prefactor in the case of a chain. In the second line, for pedagogical purposes, the same expression is written as a function of the occupations $\mathbf{n}_k$, and therefore the terms in the $C[k]$ sum that involve *changes* in the occupations (i.e., “transitions” of particles between orbitals) have been omitted. The energies of the orbitals are

$$\varepsilon_k[\text{ring}] = -K \cos(k - (\Phi/L)), \quad (14)$$

$$\varepsilon_k[\text{chain}] = -K \cos(k), \quad (15)$$

$$\varepsilon_{\text{floor}} \equiv -K, \quad (16)$$

$$\mathcal{E}_k \equiv \varepsilon_k - \varepsilon_{\text{floor}}. \quad (17)$$

In the case of a ring, the $C[k]$ coefficients restrict the summation such that $C[k] = 1$ is nonzero only if the condition $k''' + k'' - k' - k = 0$ is satisfied mod(L). In the case of a chain, all possible variations of $\pm$ signs are allowed, and $C[k]$ depends on the combination. Specifically, $C_{\text{chain}} = 3/2$ if all the k 's are identical, $C_{\text{chain}} = 1/2$ if only two k 's are identical, and $C_{\text{chain}} = 1$ if there are two different pairs. Hence, an extra $1/2$ prefactor is implied in front of the second term in Eq. (13).

Ignoring “transitions” that change the occupations of the orbitals, one concludes by inspection of Eq. (13) that for the assumed repulsion ($U > 0$) there is an energy gain due to condensation. The impression is that a finite U leads to metastability: The energy is reduced if all the particles are condensed in a single orbital. So, for a large enough U , any orbital can support an ES condensate. *This conclusion is wrong*, because the transitions are formally a “kinetic term” in the Hamiltonian that deforms the potential floor, as implied by the Bogoliubov analysis (see subsequent section). Furthermore, the implications are different for a ring and for a chain.

VI. ZERO-ORDER BOGOLIUBOV ANALYSIS

Assuming condensation in orbital “o”, and using that the number of particles is a constant of motion, we can substitute in the first term of the Hamiltonian $\mathbf{b}_{k_o}^\dagger \mathbf{b}_{k_o} = N - \sum \mathbf{b}_k^\dagger \mathbf{b}_k$. The zero-order Bogoliubov approximation is obtained if we furthermore keep only the leading terms in the interaction that

transfer *pairs* from the condensate k_o to different orbitals. For a ring, we get

$$\begin{aligned}\mathcal{H}_0[\text{ring}] &= \sum_{k \neq k_o} (\varepsilon_k - \varepsilon_{k_o} + \Delta) \mathbf{b}_k^\dagger \mathbf{b}_k \\ &+ \Delta \sum_{q>0} (\mathbf{b}_{k_o-q}^\dagger \mathbf{b}_{k_o+q}^\dagger + \mathbf{b}_{k_o-q} \mathbf{b}_{k_o+q}).\end{aligned}\quad (18)$$

For a chain, we have additional terms, notably those that create pairs in the same orbital,

$$\begin{aligned}\mathcal{H}_0[\text{chain}] &= \sum_{k \neq k_o} (\varepsilon_k - \varepsilon_{k_o} + \Delta) \mathbf{b}_k^\dagger \mathbf{b}_k \\ &+ \sum_{k \neq k_o} \Delta (\mathbf{b}_k^\dagger \mathbf{b}_k^\dagger + \mathbf{b}_k \mathbf{b}_k) \\ &+ \sum_{|k' \pm k''|=2k_o} \Delta (\mathbf{b}_{k'}^\dagger \mathbf{b}_{k''}^\dagger + \mathbf{b}_{k'} \mathbf{b}_{k''} + 2\mathbf{b}_{k'}^\dagger \mathbf{b}_{k''}) \\ &- \sqrt{N} \frac{\Delta}{2} (\mathbf{b}_{3k_o} + \mathbf{b}_{3k_o}^\dagger).\end{aligned}\quad (19)$$

The last term shifts the SP from the origin and is ignored in what we call the *zero-order* Bogoliubov analysis.

A. Ring

For a ring, the diagonalization decomposes into “blocks,” such that each block consists of two opposing orbitals, namely, $k_o \pm q$. We define the excitation energy per particle for a paired transition and the transverse excitation energy as follows:

$$\begin{aligned}\varepsilon_q^\parallel &= \frac{1}{2} (\varepsilon_{k_o+q} + \varepsilon_{k_o-q}) - \varepsilon_{k_o} = 2K \cos \frac{\phi}{L} \sin^2 \frac{q}{2}, \\ \varepsilon_q^\perp &= \frac{1}{2} (\varepsilon_{k_o+q} - \varepsilon_{k_o-q}) = K \sin \frac{\phi}{L} \sin q.\end{aligned}$$

These frequencies are conveniently expressed as a function of the unfolded phase $\phi = \Phi - 2\pi m_o$. Accordingly, without loss of generality, one assumes $m_o = 0$, gaining the option to address all the flow states in a single (ϕ, u) stability diagram. Namely, the associate Bogoliubov frequencies for a ring can be written as

$$\omega_q[\text{ring}] = \varepsilon_q^\perp + \sqrt{[\varepsilon_q^\parallel + 2\Delta]\varepsilon_q^\parallel}. \quad (20)$$

See Fig. 1 for illustration. Let us focus on a condensate that is prepared in an excited orbital in the *lower half* of the spectrum. In the absence of interactions, the Bogoliubov frequencies are *real*, but some of them are *negative*, reflecting the possibility of downward transitions. But the excitation energy $\varepsilon_q^\parallel$ for a paired transition is always *positive*. Therefore, as U increases, negative ω_q becomes positive, which implies that the condensate gets stabilized. It becomes energetically stable. An illustration for that is provided in Fig. 2(a).

B. Chain

For a chain, the diagonalization is more complicated, because we have to distinguish between several possibilities, and we end up with larger “blocks” in the diagonalization procedure. We shall provide a detailed account in the next section.

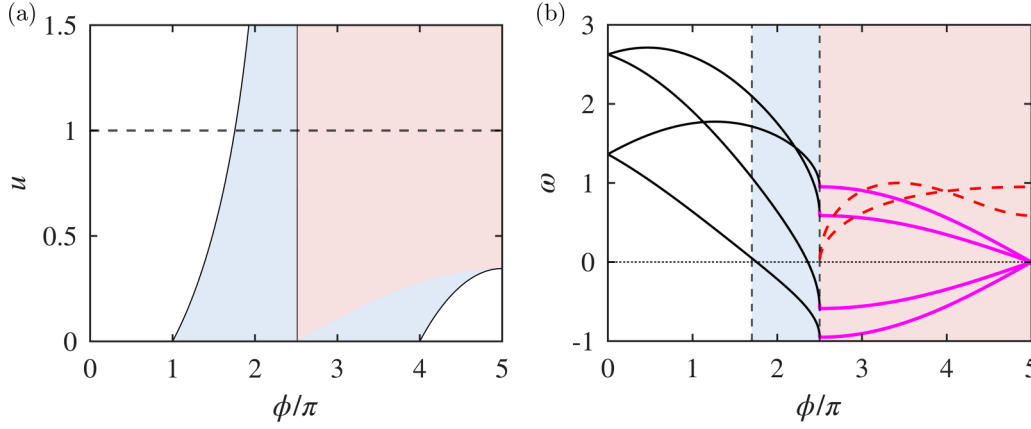


FIG. 1. Stability regimes for five-site ring. (a) The (ϕ, u) regime diagram. White regions indicate Landau energetic stability (all Bogoliubov frequencies are real and positive). Blue region indicates linear dynamical stability (Bogoliubov frequencies are real, but some become negative). Orange region indicates instability (Bogoliubov frequency becomes complex). (b) Bogoliubov frequencies along the indicated $u = 1$ section. In the region where they become complex, the real part is plotted in magenta, while the imaginary part is plotted as a red dashed line.

For pedagogical purpose, let us make the (generally incorrect) assumption that transitions between different orbitals can be ignored, keeping only the first two lines in Eq. (19). Then, the diagonalization of the Bogoliubov frequencies are

$$\omega_q[\text{chain}] = \sqrt{[\varepsilon_q^\parallel + 2\Delta]\varepsilon_q^\parallel}, \quad (21)$$

where the excitation energy per particle for a paired transition to the same orbital is simply

$$\varepsilon_k^\parallel[\text{chain}] = \varepsilon_k - \varepsilon_{k_o} = K[\cos(k_o) - \cos(k)].$$

This expression, in spite of its questionable validity, illuminates a key difference between rings and chains. For a chain, $\varepsilon_q^\parallel$ to the lower orbitals are negative. Consequently, as U increases, the Bogoliubov frequencies become *complex*, implying that the condensate becomes dynamically unstable rather than ES.

More precisely, the expression in Eq. (21) is dominated by two dimensionless parameters: the GPE parameter [Eq. (10)] and the DNLSE parameter [Eq. (11)]. For a large chain, we

first hit the GPE border and later the DNLSE border. This is illustrated in Fig. 3 and will be further discussed in the next section. Namely, one observes accumulation of negative frequencies at zero, after the GPE border is crossed, and they become complex only later, after the DNLSE border is crossed. To understand the GPE accumulation, we have to go beyond the zero-order analysis. As opposed to that, for a short chain, we encounter a premature DNLSE transition to complex frequencies, as seen in Fig. 2(b). In Appendix A, we provide the u dependence for chains with $L_s = 7, 9, 11, 13, 15, 21, 51, 91$ sites to show how the GPE limiting behavior is gradually exposed, while in Fig. 4 we show the u regions where the DNLSE instability comes into play.

VII. THE DISPLACED CONDENSATE

There is a one-to-one correspondence between quantum and the classical Bogoliubov procedure, and in practice, the latter is more transparent and more convenient. Using phase-

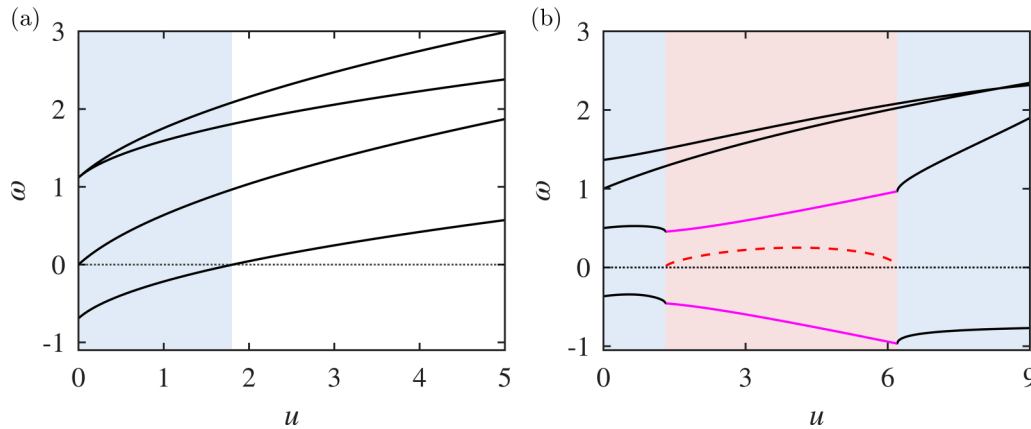


FIG. 2. Bogoliubov frequencies vs u , ring vs chain. We compare the dependence of ω_q on u for ring and chain with five sites. We inspect the SP that supports condensation in the first excited orbital. (a) The Bogoliubov frequencies ω_q for $L_s = 5$ ring. The DS to ES transition is illustrated, meaning that all frequencies become positive. (b) The Bogoliubov frequencies ω_q for $L_s = 5$ chain. In the region where they become complex, the real part is plotted in magenta, while the imaginary part is plotted as a red dashed line. The transition from DS to instability is illustrated, meaning that some frequencies become complex.

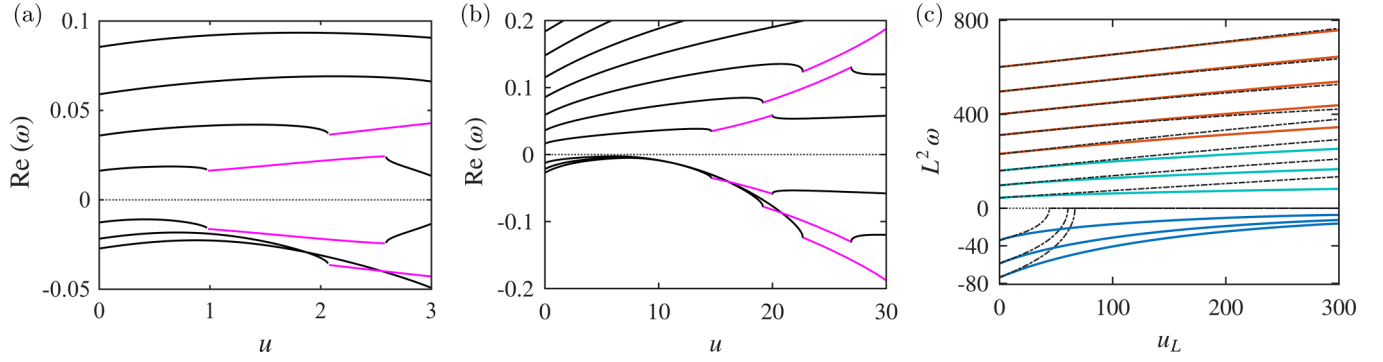


FIG. 3. Bogoliubov frequency vs u , large chain. We compare the prediction of the Bogoliubov analysis to the exact numerical calculation for a chain with 51 sites, and clarify the GPE limit for chains with many sites. We inspect the SP that supports condensation in the third excited orbital; therefore, for $u = 0$, there are three negative Bogoliubov frequencies. (a) Zero-order result. Complexity is indicated by the magenta color, as in Fig. 2, but the imaginary part is not plotted. Note that instability shows up for a relatively small value of u . (b) Exact result. Note that the transition to complexity is pushed to a large u regime, which gets excluded in the GPE limit. (c) Close-up of the GPE regime, where the frequencies are real. One observes that the negative frequencies do not change sign but rather accumulate to zero. The negative frequencies are colored in blue, and the associated low positive frequencies are colored in cyan. Additional high positive frequencies are colored in red. The thin dashed-dotted lines are the outcome of a simple-minded approximation that is explained in Appendix A.

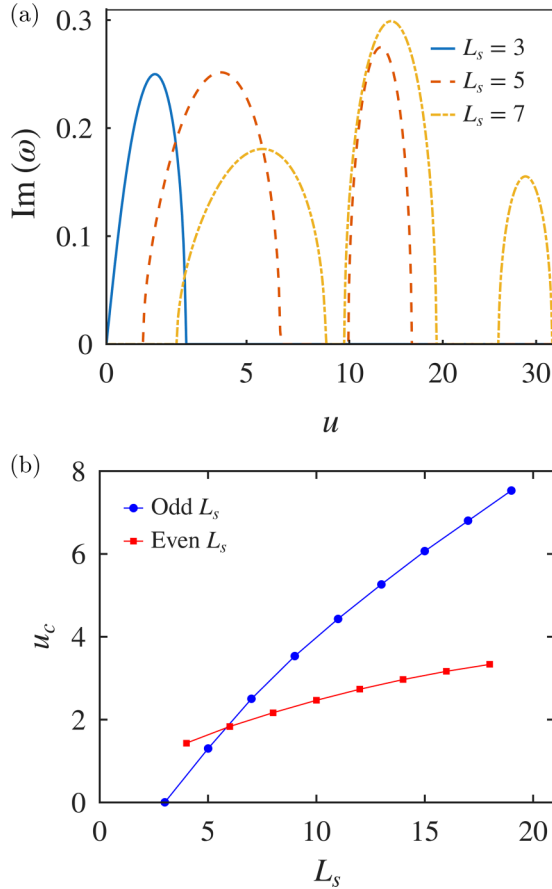


FIG. 4. Bogoliubov frequency vs u , complex frequencies. (a) The imaginary part $\text{Im}[\omega_q]$ of the Bogoliubov frequency is plotted vs u for a chain with three (blue), five (orange), and seven (yellow) sites. We inspect the SP that supports condensation in the first excited orbital. (b) The critical value u_c above which complex frequencies appear as a function of L_s . Note that for three sites $u_c = 0$. For $u_L > u_c L$, the SP becomes unstable; hence, in the GPE limit, the instability regime gets excluded, and chaos is globally diminished.

space language, the first step is to identify the SP that supports the condensate. The DNLSE is derived from the BHH via canonical Hamilton's equations using the action-angle coordinates defined in Eq. (6), and can be written as

$$i \frac{d}{dt} \psi = (\mathbf{D} + u\mathbf{P})\psi, \quad (22)$$

where $\psi = \{\psi_j\}$ is a column vector of the rescaled coordinates, namely, $\psi_j = N^{-1/2} \mathbf{a}_j$. Commonly, ψ is called *the SP wavefunction*. The definitions of the $\mathbf{D}$ and $\mathbf{P}$ matrices are implied, e.g., for the $L_s = 5$ chain,

$$\mathbf{D} = -\frac{1}{2} \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{P} = \begin{pmatrix} p_1 & 0 & 0 & 0 & 0 \\ 0 & p_2 & 0 & 0 & 0 \\ 0 & 0 & p_3 & 0 & 0 \\ 0 & 0 & 0 & p_4 & 0 \\ 0 & 0 & 0 & 0 & p_5 \end{pmatrix}, \quad (23)$$

where $p_j = |\psi_j|^2 = n_j/N$ are the rescaled occupations, such that $\sum_j p_j = 1$. The SPs of the Hamiltonian are the nonzero solutions of the equation

$$(\mathbf{D} + u\mathbf{P})\psi = \mu\psi. \quad (24)$$

The nonlinear eigenvalues can be written as

$$\mu = \varepsilon_{\text{floor}} + \Delta + \mathcal{E}, \quad (25)$$

where $\varepsilon_{\text{floor}} + \Delta$ is the potential floor and $\mathcal{E}$ is a positive “kinetic energy.” The kinetic energy in the absence of interaction is given by Eq. (17), such that $\mu = \varepsilon_k$. As further discussed

below, we can, by continuity, keep the same indexing for the nonlinear eigenvalues as the interaction is increased, though in general one can obtain additional or different nontrivial SPs via bifurcations.

For a *ring*, the trivial SP wavefunctions are *not* affected by the interaction. On the technical level, $\mathbf{P}$ is proportional to the identity matrix, and therefore the trivial zero-order SP wavefunctions remain eigenvectors of $(\mathbf{D} + u\mathbf{P})$. The only effect of the interaction is the shift of the potential floor in Eq. (25). Namely, all the μ eigenvalues are shifted by Δ , but otherwise not affected. Note that, for a ring, there are also nontrivial complex eigenfunctions [23], whose discussion is beyond the scope of the present study.

For a *chain*, the SP wavefunctions are, in general, affected by the interaction. The simplest example is the SP wavefunction of an $L_s = 7$ chain that supports the $m_o = 2$ condensate. For zero interaction, $\psi \propto \sin(kx)$ with $k = (\pi/8)m_o$, while for very large u the wavefunction gets flattened except the zero at the $x = 4$ node. The associated densities are

$$\mathbf{p}|_{\text{zero } u} = \{|\psi_j|^2\} = \frac{1}{8}\{1, 2, 1, 0, 1, 2, 1\}, \quad (26)$$

$$\mathbf{p}|_{\text{large } u} = \{|\psi_j|^2\} \approx \frac{1}{6}\{1, 1, 1, 0, 1, 1, 1\}. \quad (27)$$

More generally, for larger L_s , in the GPE limit, there is a nodal structure that does not change with the interaction. Namely, the stationary solutions deform smoothly as the interaction is increased. For small u they look like sinusoids, while for larger u they become elliptic functions. For very large u , the density $p_j = |\psi_j|^2$ becomes uniform, interrupted by dark solitons at the nodes. Nodes neither disappear nor are generated. Based on Eq. (24) of Ref. [23], one obtains

$$\mathcal{E}|_{\text{zero } u} = \frac{K}{2} \left(\frac{\pi}{L} m_o \right)^2, \quad (28)$$

$$\mathcal{E}|_{\text{large } u} \approx 2K \frac{\sqrt{uL}}{L^2} m_o. \quad (29)$$

One observes that the crossover from the small to the large u regime happens at the GPE border of Eq. (10). The equal spacing for large u reflects the cost of each soliton notch.

Once we find the SP wavefunction, we can also calculate the optional n_k coordinates from its n_j coordinates. In particular, the SP wavefunctions of a chain in the GPE limit feature approximately uniform density for large u ; hence, we get

$$\frac{n_k}{N} \approx \frac{8}{\pi^2} \left(\frac{k_o}{k} \right)^2, \quad (30)$$

where k should be an odd harmonic of k_o . We use the notation $n_{\text{SP}} \equiv n_{k_o}$. For a nondepleted condensate, $n_{\text{SP}} = N$. For strong interaction, we get from the above formula $n_{\text{SP}} \approx 0.8N$, meaning that even for very large u , the depletion of the condensate is no more than 20%. We can also calculate E_{SP} . Based on Eq. (13), one obtains

$$E_{\text{SP}} = \varepsilon_{k_o} N + \frac{3U}{4L} N^2. \quad (31)$$

If we go beyond zero order, the SP might become shifted such that $n_o = n_{\text{SP}}$ is less than N . If this is the case, it means that the stationary condensate is somewhat depleted. Accordingly, in

the quantum treatment, the condensate is semiclassically represented by a Gaussian-like cloud that might be both *shifted* and *squeezed* relative to the zero-order solution.

VIII. EXACT BOGOLIUBOV ANALYSIS

This section is rather technical and can be skipped in the first reading. In the next section, we discuss the implied stability regimes for rings and chains, which provide a bridge to the tomographic inspection of the spectrum.

For the purpose of stability analysis, one finds the Bogoliubov frequencies ω_q of the small oscillations around the SP. For that purpose, one has to carry out the diagonalization of the Bogoliubov matrix $\mathbf{W}$, which is obtained from the Hessian of the Hamiltonian $\mathcal{H}(a, \bar{a})$. For a chain and also for a nonrotating ring, the SP wavefunction ψ is real, and $\mathbf{W}$ can be written as follows:

$$\mathbf{W} = \begin{pmatrix} \mathbf{D} + 2u\mathbf{P} - \mu & -u\mathbf{P} \\ u\mathbf{P} & -(\mathbf{D} + 2u\mathbf{P} - \mu) \end{pmatrix}. \quad (32)$$

The diagonalization results in L_s pairs of characteristic frequencies $\pm\omega_q$, which are indexed by q . The trivial frequency $\omega_0 = 0$ is implied by conservation of particles.

The zero-order Bogoliubov analysis assumes that the SP for $u > 0$ is the same as the SP of the noninteracting system. We already pointed out that this assumption is correct for the trivial SP wavefunctions of the ring. Namely, the uniform density of the condensed particles is not affected, and therefore the ω_q of Eq. (20) are exact.

The zero-order Bogoliubov analysis is also exact for the middle orbital of a chain with an odd number of sites (see Appendix B). But this is not very interesting because only the lower half of the spectrum survives in the GPE limit. The upper half of the spectrum formally corresponds to bosons with attractive interactions, which is not of our interest here. In the following, we discuss the results for ω_q for condensation in orbitals that belong to the lower half of the spectrum.

A. Chain with five sites

For a general chain, the SPs that support the $u = 0$ condensates are displaced once the interaction is turned on. Conveniently, this is not the case with the SP wavefunction $\psi^{(1)}$ that supports the first excited orbital of the five-site chain. This SP is not displaced by the interaction

$$\psi_j^{(1)} = \frac{1}{2}(1, 1, 0, -1, -1). \quad (33)$$

The five-site chain is going to serve as our leading numerical illustration; therefore, we provide here explicit expressions for the Bogoliubov frequencies. They are indexed as $q = -1, 0, 1, 2, 3$. Two roots (ω_0 and ω_2) are rather trivial, while the other three are determined by a cubic equation (see Appendix B). The result is

$$\omega_{\pm 1}^2 = \frac{1}{3} \left(c_2 + e^{\pm i\pi/3} C + e^{\mp i\pi/3} \frac{\Delta_0}{C} \right), \quad (34)$$

$$\omega_2^2 = 1 + \frac{1}{2}u, \quad (35)$$

$$\omega_3^2 = \frac{1}{3} \left(c_2 + C + \frac{\Delta_0}{C} \right). \quad (36)$$

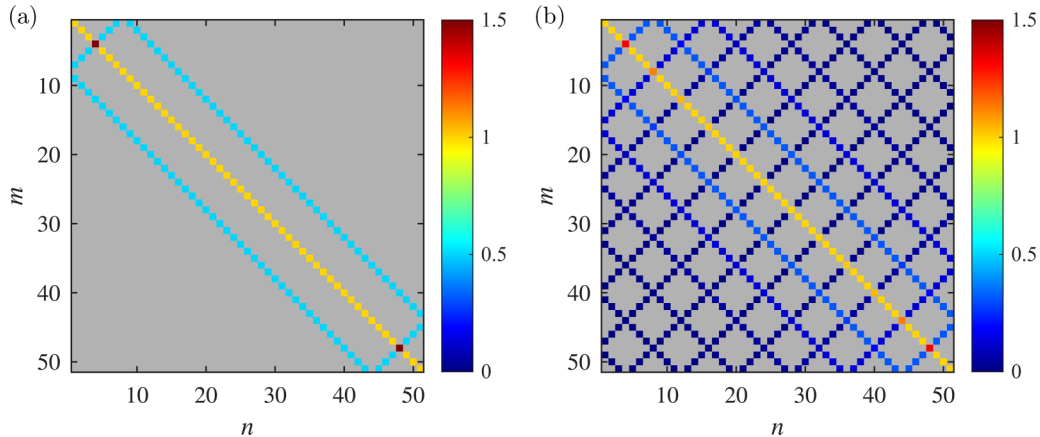


FIG. 5. The structure of the $\tilde{\mathbf{P}}$ matrix. Image of the $\tilde{\mathbf{P}}$ matrix (multiplied by $L = L_s + 1$) in the orbital representation for the $m_o = 4$ stationary state of an $L_s = 51$ chain. Left and right panels are for $u = 0$ and $u = 8$. Exact zero values are colored in gray, while blue color indicates very small nonzero numerical values.

For small u , C comes out negative and consequently the frequencies come out real. The critical value $u_c \approx 1.307$ is the minimal u that makes $\omega_{\pm 1}$ complex. The dependence of the Bogoliubov frequencies on u is plotted in Fig. 2(b). As opposed to the ring, here, as u is increased, we have a transition to instability instead of a transition to ES.

B. Chain with many sites

In general, the SP of a chain is affected by u . Consequently, the zero-order Bogoliubov results are flawed. The exact calculation requires first finding the SP wavefunction and then calculating $\mathbf{P} = \text{diag}\{\mathbf{p}\}$. It is illuminating to transform this matrix into the orbital representation. An illustration is provided in Fig. 5. For zero interaction, the nonzero elements are in one-to-one correspondence with the bilinear terms of Eq. (19). As u is increased, the off-diagonal elements get smaller, but on the other hand, a pattern appears that reflects the comb of notches that is featured by the solitonic stationary distribution.

The failure of the zero-order approximation is demonstrated numerically in Fig. 3, where we plot [panel (a)] the prediction that is based on the zero-order Bogoliubov analysis. The ω_q becomes complex as u becomes of order unity. But in the exact calculation [panel (b)], this happens for a much larger value of u . We enlarge the GPE regime where the frequencies are real [panel (c)]. The outcome of a simple-minded approximation that is based on blockwise diagonalization of $\mathbf{W}$ is indicated by thin dashed-dotted lines. Its reasoning is explained in Appendix A. It provides expressions of the type provided in Eqs. (20) and (21). It fails to deliver a proper explanation for the accumulation of the negative frequencies.

In order to explain the accumulation of the negative frequencies, it is better to take a second look at $\mathbf{W}$ of Eq. (32) as written in the site representation. If we ignore pair destruction and creation, the eigenfrequencies are obtained from the diagonalization of the GPE-like block, where the mean-field potential is enhanced by a factor 2, and shifted by μ . If this potential were flat, we would get $\omega_q(u) = \omega_q(0) + \Delta$,

reflecting the extra cost Δ for relocating a particle from the k_o orbital to a different orbital. But the mean-field potential has notches where the potential is $-\Delta$. Those notches can support eigenvectors that have negative frequencies. These frequencies become less negative as u increases, because we have to add the kinetic energy that comes from $\mathbf{D}$. This kinetic energy is bounded by unity (which means K in unscaled units). Hence, as we come close to the GPE border of Eq. (10), the kinetic energy of the eigenvectors compensates the Δ , leading to close-to-zero frequencies. There are, of course, the pair destruction/creation terms that couple the two blocks of $\mathbf{W}$. Their effect is similar to what we have encountered in the calculation for a ring. They mainly affect the positive frequencies, and we can use the simple-minded approximation as discussed in Appendix A.

Still, one wonders whether it is possible to obtain a tangible approximation for the negative frequencies. This goes beyond the scope of our interest here, but we point out the following hand-waving estimate. If we had an infinite chain, the notch would gain translational symmetry, meaning that the “negative” frequencies are in fact Goldstone modes with zero frequency. But if we have a comb of notches distance L/m_o apart, we expect negative frequencies of order $\exp[-L/(m_o\xi)]$ due to tunnel overlap.

IX. STABILITY REGIMES

On the basis of the previous section, let us discuss the implications with regard to the stability of a given SP. If all the Bogoliubov frequencies are real and positive, then the SP is a stable minimum (ES). If some are negative (but real), it indicates that the SP is a stable elliptic point that sits on a saddle in the energy landscape, suggesting DS. If some of the frequencies become complex, it indicates that the SP is an unstable hyperbolic point, and possibly it is associated with the emergence of chaos in its vicinity.

A. Ring

For a ring, a given orbital, indexed as $k_o = 2\pi m_o$, constitutes a trivial SP in phase space: Its location is not affected

by the interaction because the particles are distributed uniformly over the sites. The stability diagram for $L = 5$ was displayed in Fig. 1. For pedagogical purpose, we consider a section along $u = 1$. As ϕ is increased, the $m_o = 0$ condensate becomes metastable once $\phi > \pi$. Then, at ϕ_c^{ES} it goes from ES to DS, and after that at ϕ_c it goes from DS to instability.

Let us expand on the determination of the borders between the stability regimes. If the ring is large ($L \gg 1$), an approximation for Eq. (20) is $\omega_q \approx c_s|q| + v_o q$, where $c_s = \sqrt{NUK/L}$ is the speed of sound and $v_o \approx (K/L)\phi$. Recall that $\phi = \Phi - 2\pi m_o$; hence, v_o is the rotation velocity of the ring *relative* to the superflow. Consequently, we deduce the Landau criterion for stability $|v_o| < c_s$, leading to $|\phi| < \phi_c^{\text{ES}}$, where

$$\phi_c^{\text{ES}} = \sqrt{uL}. \quad (37)$$

It ensures that all the excitations in the rotating frame are positive, and hence the SP is a local minimum.

More generally, if L is not large, the generalized Landau criterion for ES involves the lowest excitation frequency ω_q that is obtained for $|q| = 2\pi/L$. Hence, we get

$$2 \cos\left(\frac{\phi_c^{\text{ES}}}{L}\right) = -\left(\frac{u}{L}\right) + \sqrt{\left(\frac{u}{L}\right)^2 + 4 \cos^2\left(\frac{q}{2}\right)}. \quad (38)$$

Consistency, with the large L approximation is easily verified. Given L , the critical value ϕ_c^{ES} increases with u from the minimal value $\phi_c^{\text{ES}} \sim \pi$ to the limiting value $\phi_c^{\text{ES}} \sim (L/2)\pi$. Irrespective of that, the Bogoliubov frequencies become complex once the stability border ϕ_c is crossed. Namely, we get the following sequence of transitions:

$$\pi < \phi_c^{\text{ES}}(u) < \phi_c = L\frac{\pi}{2}. \quad (39)$$

Optionally, we can consider a nonrotating ring. In Fig. 2(a), we plot the ω_q of the $m_o = 1$ excited condensate as a function of u . As the interaction increases, $\phi_c^{\text{ES}}(u)$ becomes larger than ϕ , and consequently, the negative Bogoliubov frequency becomes positive, and the stability of the condensate changes from DS to ES.

B. Chain

We now ask what happens if we have a chain instead of a ring. The dimensionless parameters that control the stability analysis are Eqs. (10) and (11). As already discussed in previous subsections, the GPE and the DNLSE parameters determine, respectively, borders that indicate the accumulation of negative frequencies, and for getting instability. This was illustrated in Fig. 3. For short chains, the DNLSE border comes before the GPE border, and then the GPE region is not exposed, and no accumulation is observed, as was demonstrated in Fig. 2(b).

For the purpose of comparison between chains and rings, let us consider a nonrotating ring ($\Phi = 0$). Then, the relative velocity of the superflow is $|v_o| = (K/L)2\pi|m_o| = Kk_o$. As u is increased, the stability changes from DS to ES. See illustration in Fig. 2(a) for an $L_s = 5$ ring. In the GPE regime, we write again the Landau criterion

$$|v_o| < c_s, \quad (40)$$

where v_o is the flow velocity. For a chain, the analogous definition would be $v_o = Kk_o = K(\pi/L)m_o$. Recalling that $c_s = \sqrt{uL}K/L$, it follows that the stability border that is implied by the Landau criterion coincides with the GPE border of Eq. (10).

We therefore conclude that the Landau stability border coincides with the GPE border. For a ring, the negative frequencies change sign, and we get ES. For a chain, they do not change sign but rather accumulate to zero.

The GPE regime is furthermore bordered by DNLSE instabilities. For an $L_s = 5$ chain, we saw in Fig. 2(b) that as u is increased, there is a transition at u_c from DS to instability. Looking further, we see that for much larger u , we get DS again. More generally, for the first excited orbital for chains of length $L_s = 3, 5, 7$, we get the results that are displayed in Fig. 4 featuring several DS regions.

For long chains, the DNLSE border is pushed to much larger values of u , hence exposing a fully developed GPE-like regime. Looking in Fig. 4(b), one observes that for a chain with an even number of sites, the critical value is smaller. This shows that for an even number of sites, the SP wavefunction ψ does not have a node and is therefore somewhat more uniform. Irrespective of that, we see that for large L_s we get $u_c = \infty$; hence, the critical value of $u_L = u_c L$ goes to infinity *faster than* L , meaning that all the condensates are DS in the GPE limit.

X. CLASSICAL TRAJECTORIES

Having diagnosed whether an SP is stable or not, we now zoom out and want to know whether it is located within a stable island or embedded in a chaotic sea. For this purpose, we inspect long trajectories that are launched either in the vicinity of the SP or somewhere else, away from the SP, but at the same energy. Representative trajectories are plotted in Figs. 6, 7, and 9 for $L_s = 3, 5, 51$ chains. We discuss the figures in the following paragraphs.

The $L_s = 3$ chain is somewhat nongeneric because it features SP instability for arbitrarily small u . Nevertheless, we see that for weak interaction ($u = 0.5$) the motion is quasiregular, and only for stronger interaction ($u = 1.5$) it becomes chaotic. This is clear by inspection of Figs. 6(a) and 6(b), but also can be quantified via Fourier analysis (power spectrum of the motion) or via Lyapunov analysis (see later section). In the chaotic regime, we observe ergodicity, meaning the loss of “memory” of the initial conditions. Strangely enough, as we further increase the interaction ($u = 3.5$) [see Fig. 6(c)], a stability island is born, well separated from the chaotic sea. This is inverse to the DS-to-instability transition.

The $L_s = 5$ chain is rather generic. For small interaction ($u = 0.5$), the motion is quasiregular, and the SP is dynamically stable [see Fig. 7(a)]. For strong interaction ($u = 3.5$), the motion is chaotic, the SP is dynamically unstable, and one observes ergodicity [see Fig. 7(c)]. Nevertheless, this system has more than 2 dof. Therefore, the topology of phase space does not allow the existence of a strictly isolated island. In principle, one expects Arnold diffusion. However, such a type of escape is very slow (exponentially large with respect to the perturbation) and therefore cannot be observed in practice. What we can do is to lower the interaction to a

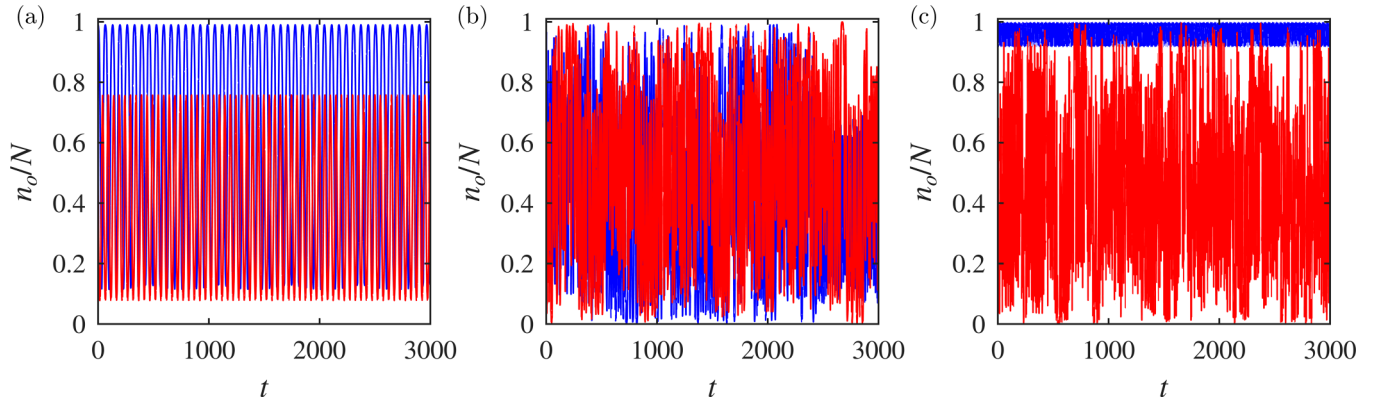


FIG. 6. Representative classical trajectories for three-site chain. The trajectories are launched at $n_o/N = 1$ (blue) and at $n_o/N = 0.5$ (red). Plot of n_o/N vs time, from left to right: (a) $u = 0.5$ (quasiregular phase space that contains an unstable SP); (b) $u = 1.5$ (chaotic phase space that contains an unstable SP); and (c) $u = 3.5$ (separated chaotic sea and stable SP island).

value that is still larger but very close to the critical value ($u_c = 1.3$). Indeed, for $u = 1.5$, we see in Fig. 7(b) that the trajectory launched at the SP eventually escapes, indicating ergodicity.

In order to gain a more quantitative perspective on the route toward ergodicity, we plot in Fig. 8 the long-time expectation value $\langle n_o \rangle$ versus the initial $n_o(t = 0)$. We see that the lack of ergodicity is reflected in the quasiregular regime [panel (a)]. In the ergodic regime [panel (b)], the expectation value $\langle n_o \rangle$ depends only weakly on the initial n_o . In contrast, we see how the existence of a stability island is reflected in the DS regime [panel (c)]. The crossover (as a function of u) is affected by the practical limitation on the time of the simulation. As already pointed out, the time for Arnold-type ergodication is exponentially large, and therefore would not be observed even if Nature were classical. For a quantum system, such long timescales are totally irrelevant because they exceed the Heisenberg time.

Representative trajectories for a long chain ($L_s = 51$) are presented in Fig. 9. Here, the SP is displaced. If the trajectory is launched very close to the SP, the motion is bounded and involves essentially a single mode. If the launching point is further away from the SP, we observe a crossover from quasi-integrability to chaos. An additional observation is that even

in the latter case, chaos in a large chain, the motion actually involves a rather small number of modes.

XI. SPECTRUM TOMOGRAPHY

A tomographic image of the spectrum provides insight into the underlying phase-space structure that supports the quantum eigenstates. The following figures display quantum tomographic images of the spectrum (panels of the third column), which are compared with classical tomography (panels of the first and second columns). Figure 10 is for an $L_s = 5$ ring, Fig. 11 is for an $L_s = 3$ chain, and Fig. 12 is for an $L_s = 5$ chain.

Each point in the quantum tomographic image represents an eigenstate, whose vertical position is the energy E_v . The extra dimensions (horizontal axis and color code) are exploited to reveal properties of the eigenstates. Here, specifically, the horizontal axis and the color code correspond, respectively, to the occupation of an inspected orbital labeled as “o” and to the purity of the eigenstate. Namely, each eigenstate is represented by a point $(E_v, \langle n_o \rangle_v)$ that is color coded by $\mathcal{S}_v$. For the ring, we inspect, without loss of generality, the $m = 0$ orbital, which becomes an excited orbital once $\phi > \pi$. For the chains, we inspect the first excited orbital ($m = 2$).

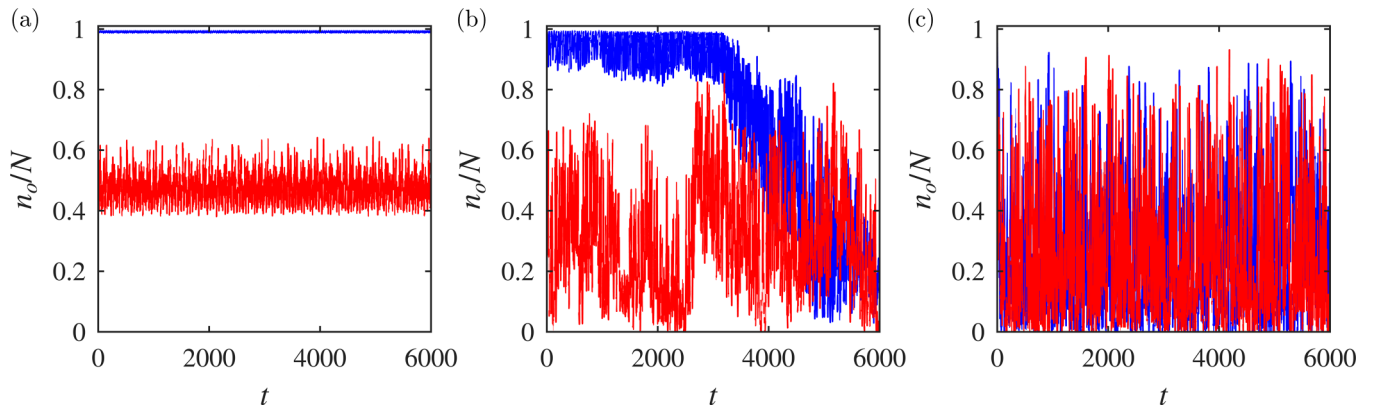


FIG. 7. Representative classical trajectories for five-site chain. The trajectories are launched at $n_o/N = 1$ (blue) and at $n_o/N = 0.5$ (red). Plot of n_o/N vs time, from left to right: (a) $u = 0.5$ (quasiregular phase space that contains stable SP); (b) $u = 1.5$ (just after the stability threshold $u_c \approx 1.3$); and (c) $u = 3.5$ (chaotic phase space that contains unstable SP).

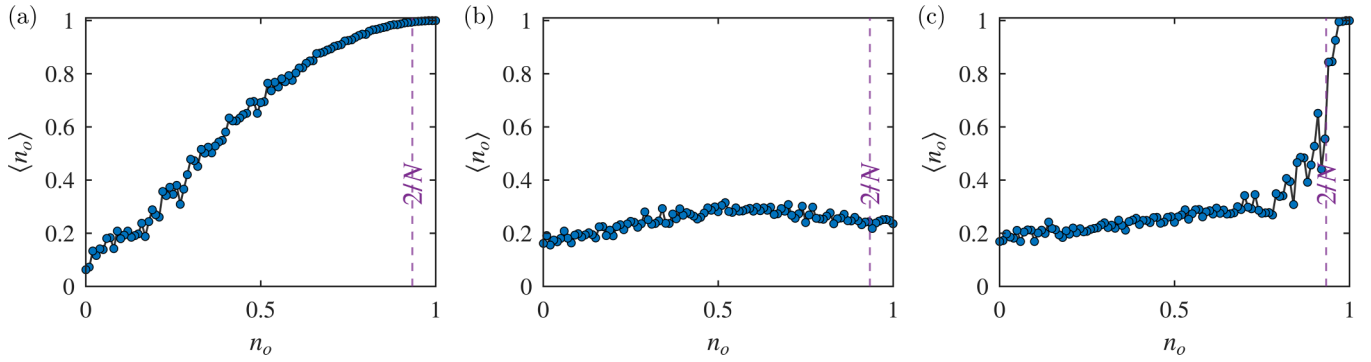


FIG. 8. The stability island for five-site chain. The size of the stability island is determined via classical simulations. The trajectory is launched at n_o , and after a long run, the average of n_o is calculated. We consider $L_s = 5$ chain with (a) $u = 0.5$ (quasiregular phase space that contains stable SP), (b) $u = 3.5$ (unstable SP that is contained in a chaotic sea), and (c) $u = 7.5$ (stable SP separated from the chaotic sea). The quantum uncertainty border $2/N$ for $N = 30$ is indicated by the vertical dashed line, implying that the stability island in the second stability range is barely resolved by the quantum eigenstates.

The quantum spectrum is obtained via diagonalization of the Hamiltonian matrix, which is a rather cheap procedure from a numerical perspective. We compare it to the classically generated spectrum. The latter is numerically expensive. It is obtained as follows: We select a large random set of points in phase space, and then use a representative subset of the points as initial conditions for long trajectories. For each trajectory, we calculate the temporal average of $n_o(t)$, which we regard as the classical analog of $\langle n_o \rangle_v$. Then, we construct a classical tomographic image of the spectrum by plotting a point $(E, \langle n_o \rangle)$ for each trajectory.

A. Ring

The first row of Fig. 10 illustrates ES of the inspected condensate. For $\phi = 1.1\pi$, the metastable eigenstate is located

in a local minimum. The minimum is shallow, and therefore, for presentation purpose, we chose a rather strong interaction ($u = 4$) that allows reasonable resolution. For this value of u , the upper part of the spectrum is chaotic, and due to ergodicity $\langle n_o \rangle$ is roughly the same for all initial conditions at the same energy. The dispersion merely reflects that our “long” trajectories have a finite time duration. The uppermost eigenstates are self-trapped states, hence featuring $\langle n_o \rangle = N/5$.

The second row of Fig. 10 ($\phi = 2.1\pi$) illustrates DS of the inspected condensate, while in the third row ($\Phi = 2.7\pi$) the SP is unstable, and therefore a metastable condensate does not exist. However, $u = 1$ is a rather low value, and therefore ergodicity is not achieved. The spread of $\langle n_o \rangle_v$ reflects the underlying quasiregular structure of phase space. In order to demonstrate ergodicity due to chaos for the same ϕ , we display in the fourth row the spectrum for $u = 4$.

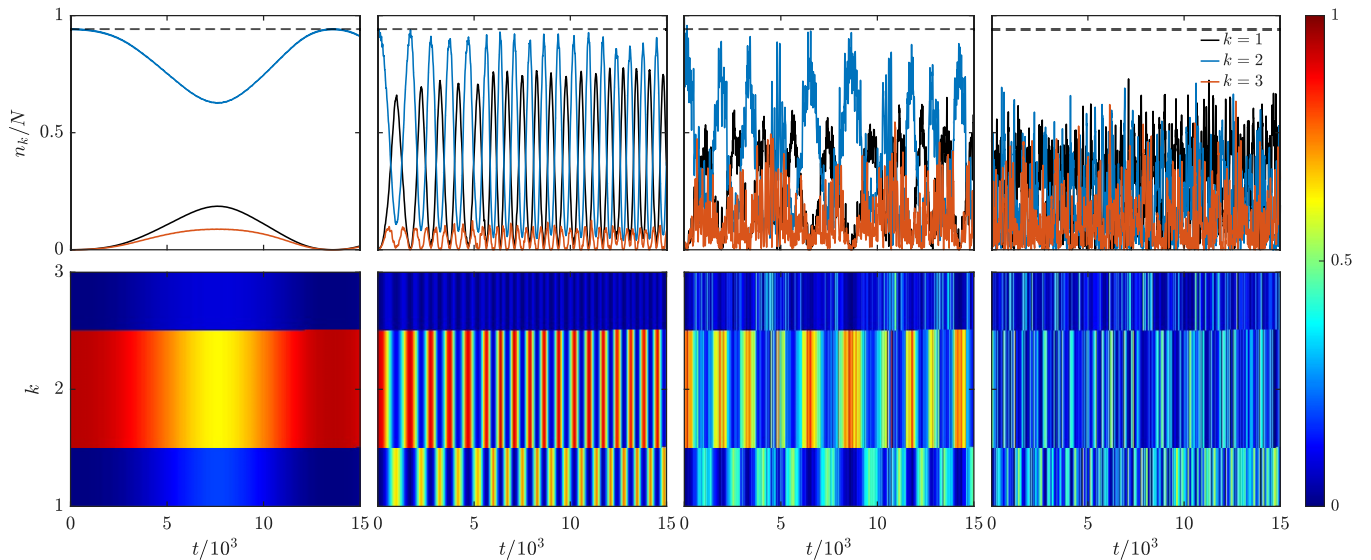


FIG. 9. Representative classical trajectories for 51-site chain. The nonvanishing coordinates n_k are plotted as a function of time. The lower panels show the same plots in image format. The interaction is $u = 5$. In the legend, “ $k = 1, 2, 3$ ” means $k = (\pi/L)m$ with $m = 1, 2, 3$. The dashed horizontal line $n_{\text{SP}}/N = 0.94$ indicates the location of the $m = 2$ SP. This value reflects the depletion of the condensate due to the solitonic deformation of the SP wavefunction. The trajectories are launched in the vicinity of this SP with a displaced value for the n_o coordinate. From left to right: $n_o/N = 0.94$ and $n_o/N = 0.93$, and $n_o/N = 1.0$ and $n_o/N = 0.45$. Note that the other coordinates are rescaled such that $\sum n_k = N$.

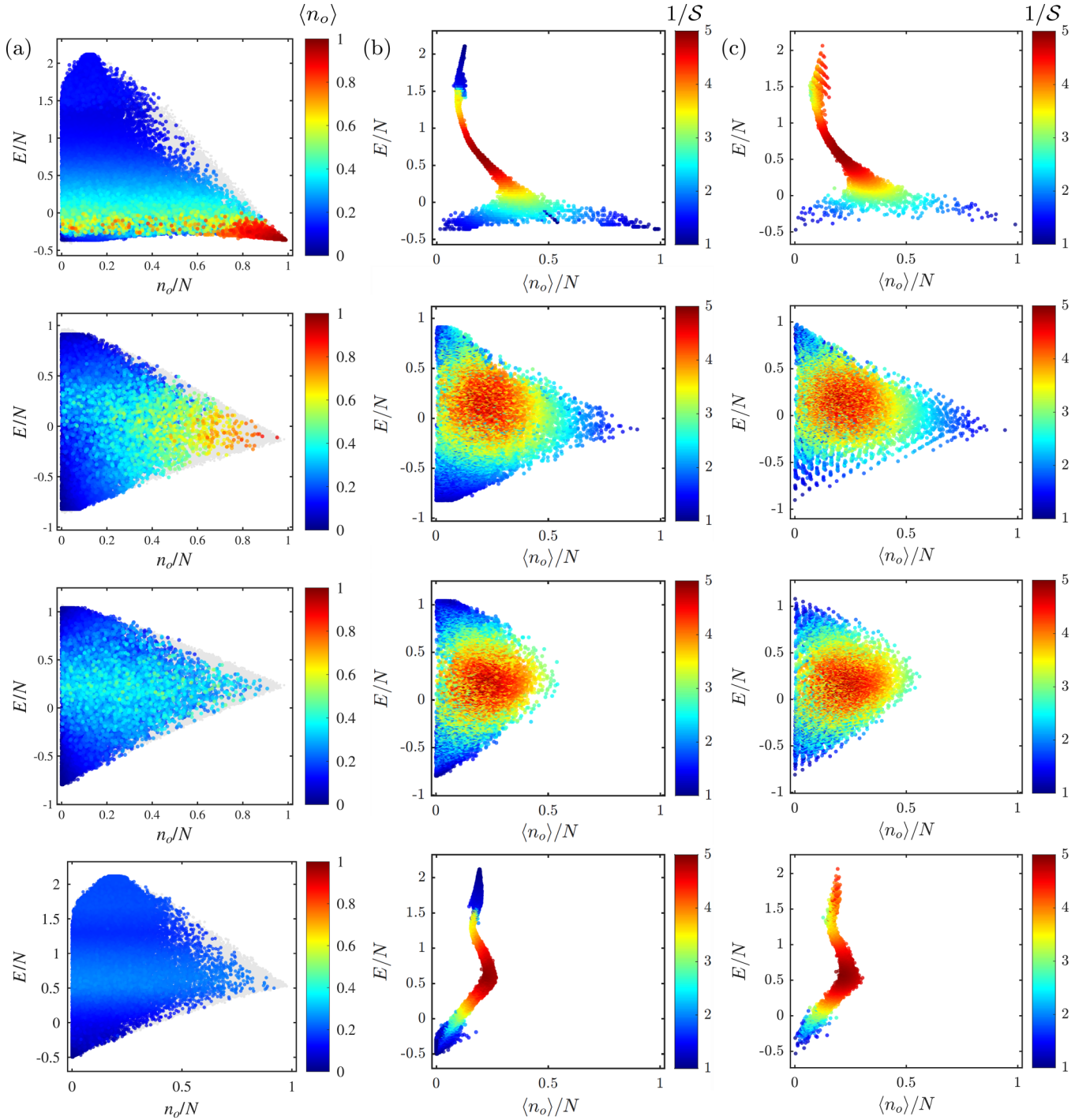


FIG. 10. Tomographic spectra for a five-site ring. The columns are for (a) classical (n_o, E) energy landscape. The plots display a uniform distribution of phase-space points (E, n_o) . Some of the points are used as initial conditions for a long trajectory of duration $t = 2500$, and color coded according to the temporal average $\langle n_o \rangle$. (b) Classical $(\langle n_o \rangle, E)$ spectrum, color coded by inverse classical purity $1/S$. (c) Quantum $(\langle n_o \rangle, E)$ spectrum for $N = 30$ particles, color coded by inverse purity $1/S$. Only $P = 0$ eigenstates are included. The rows from top to bottom are for $(u = 4, \phi = 1.1\pi)$ demonstrating ES of the SP; $(u = 1, \phi = 2.1\pi)$ demonstrating DS of the SP; $(u = 1, \phi = 2.7\pi)$, where the SP becomes unstable; and $(u = 4, \phi = 2.7\pi)$, where, due to the increased chaos, we get ergodicity, similar to as seen in the upper part of the first-row spectrum.

B. Chain

Figure 11 displays tomography for an $L_s = 3$ chain with $N = 150$ particles. Recall that such a chain is nongeneric. For small interaction ($u = 0.5$), the SP is unstable, but the

dynamics is quasiregular. For stronger interaction ($u = 1.5$), chaos is still rather weak, and therefore ergodization is poor. For strong interaction ($u = 3.5$), the chaos is strong enough to induce ergodization in the chaotic sea, but on the other hand, the SP gains DS; hence, we have an island of stability. The

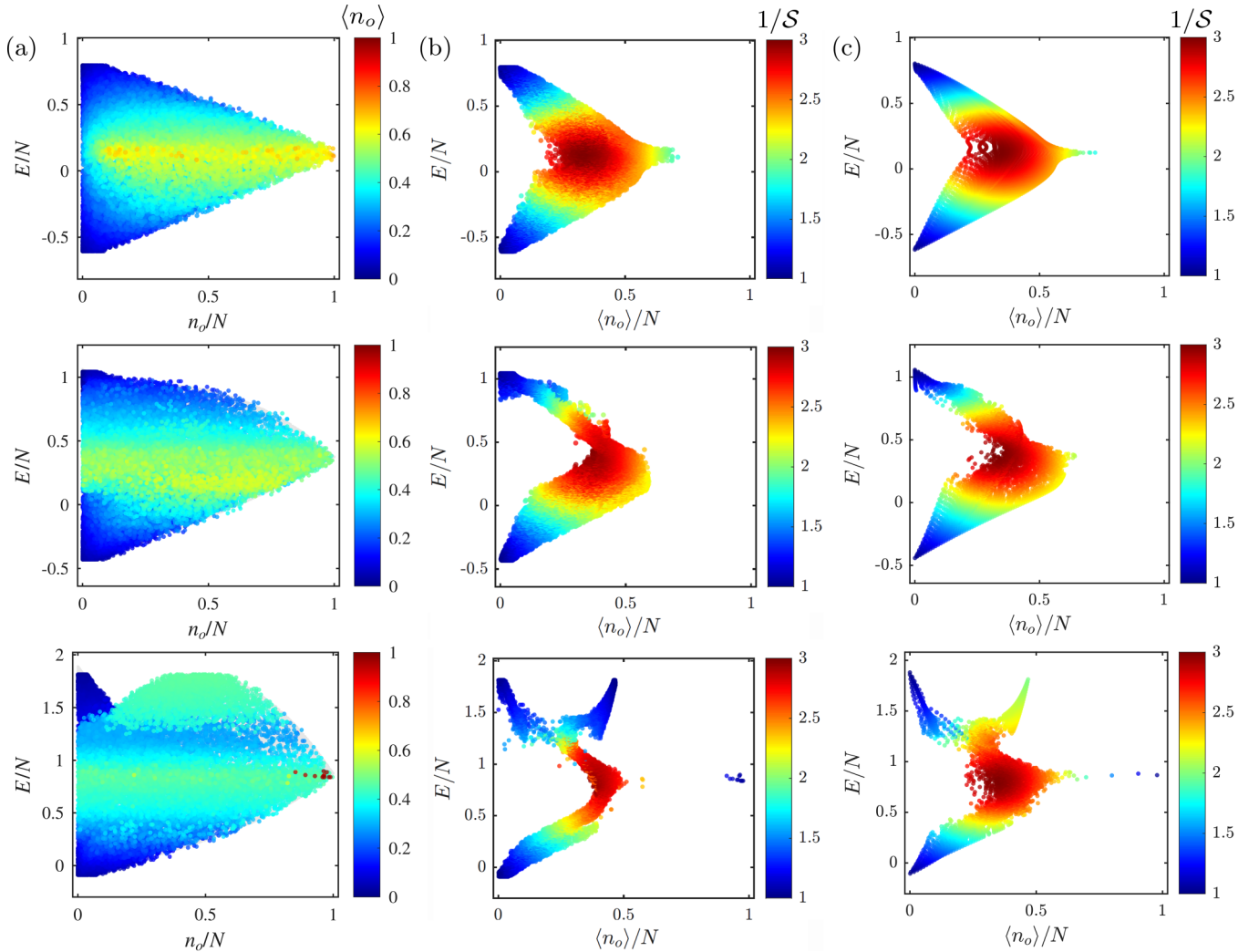


FIG. 11. Tomographic spectra for a three-site chain. The columns are arranged as in Fig. 10: (a) energy landscape, (b) classical spectrum, and (c) quantum spectrum. In column (c), the spectrum is for $N = 150$ particles, and odd-parity states are excluded. The rows from top to bottom are for $u = 0.5$ (quasiregular phase space that contains an unstable SP), $u = 1.5$ (chaotic phase space that contains an unstable SP), and $u = 3.5$ (separated chaotic sea and stable SP island).

quantum spectrum features *hybrid* eigenstates and therefore the sea/island classification is blurred. In the upper part of the spectrum, self-trapping in the middle site is conspicuously distinguished from self-trapping in the two opposing sites.

Figure 12 displays tomography for an $L_s = 5$ chain with $N = 30$ particles. This is our *generic* example for a chain. It exhibits a GPE-like DS regime for weak interactions, which is demonstrated with $u = 0.5$ in the upper row. Irrespective of that, the dynamics is quasiregular. For stronger interaction ($u = 3.5$), the SP becomes unstable, and due to chaos, we get ergodicity. The upper part of the spectrum reflects self-trapping. For larger interaction ($u = 7.5$), the SP becomes again DS, which is the same scenario as discussed for the $L_s = 3$ ring. But here the quantum spectrum does not follow the classical spectrum. The stability island is too small to be resolved, and a DS condensate does not appear. The reason for this is the small value of N . In Fig. 8, we show that the uncertainty width is comparable with the size of the stability island, and apparently the latter is too small to accommodate an eigenstate.

The above tomography illuminates generic features of *high-dimensional chaos*. The ergodicity within the chaotic sea becomes much better, which is reflected in the very narrow dispersion of $\langle n_o \rangle$. Consequently, the stability island is better resolved: It is a well-separated tiny region with $\langle n_o \rangle \sim N$. At the same time, its borders become ill-defined topologically, as discussed in connection with Fig. 8 in Sec. X.

XII. SPECTRAL FINGERPRINTS OF METASTABILITY

We would like to inspect quantitatively whether or how the stability of the SP is reflected in the tomography of the quantum spectrum. For demonstration, we use the following procedure. Given a tomographic $(\langle n_o \rangle, E)$ spectrum, the subscript “max” is used to indicate the many-body eigenstate $|E_v\rangle$ for which $\langle n_o \rangle_v$ is maximal. The values of $\langle n_o \rangle_v$ and $\mathcal{S}_v$ for this state are denoted as $n_{\max}$ and $\mathcal{S}_{\max}$. If $u = 0$, we get $n_{\max} = N$ and $\mathcal{S}_{\max} = 1$. We discuss below what happens for reasonably large u .

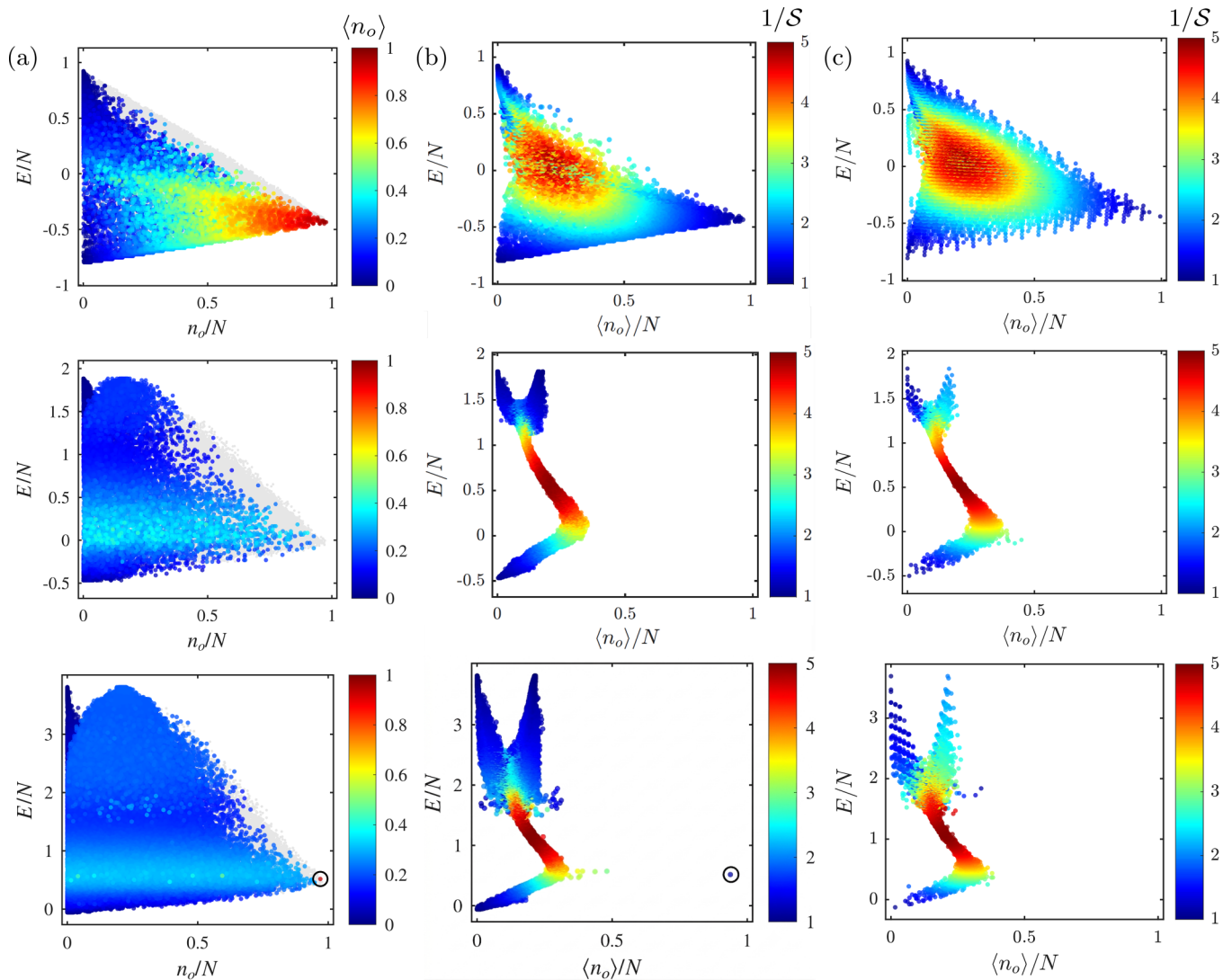


FIG. 12. Tomographic spectra for a five-site chain. The columns are arranged as in Fig. 10: In column (c), the spectrum is for $N = 30$ particles, and odd-parity states are excluded. The rows from top to bottom are for $u = 0.5$ (quasiregular phase space that contains stable SP), $u = 3.5$ (chaotic phase space that contains unstable SP), and $u = 7.5$ (separated chaotic sea and stable SP island). For weak interaction, there is no indication of chaos, and we identify a dynamically stable condensate. For stronger interaction (second and third rows), the ergodization is an indication of chaos, and in the upper part of the spectrum, one identifies self-trapping. In the third row, the quantum spectrum fails to resolve the stability island (encircled in the left panels, with no corresponding eigenstate in the right panel).

A. Ring

Let us focus on the five-site ring. As the control parameter ϕ is varied, the condensate experiences $\text{ES} \rightsquigarrow \text{DS} \rightsquigarrow \text{instability}$ transitions. We label the inspected orbital by “o”. Here, “o” refers to the $m = 0$ orbital. The dependence of $n_{\max}$ and $\mathcal{S}_{\max}$ on ϕ is presented in Fig. 13 for $u = 1$ and for $u = 4$. Up to $\phi = \pi$, the inspected condensate is trivially stable, simply because it is the ground state. For larger ϕ , we still have ES up to $\phi = 1.75\pi$. Then, we observe a moderate drop in $n_{\max}$. Once ϕ crosses the instability threshold at $\phi = 2.5\pi$, there is a much sharper drop, indicating that the metastable condensate has been diminished. Note that for the larger value of u , it is difficult to resolve the two transitions.

Subsequently, for $u = 1$, there is recovery of the stability as the $m = 0$ orbital approaches the top of the energy landscape. This recovery becomes obvious once we notice

that, for $\Phi > 4\pi$, the top state is in fact the ground state of the $U \mapsto -U$ Hamiltonian. The latter features a self-trapping transition for large u ; hence, recovery is avoided. This self-trapping was also apparent in the tomographic spectrum.

B. Chain

The dependence of $n_{\max}$ and $\mathcal{S}_{\max}$ on u for a three-site chain and for a five-site chain is presented in Fig. 14. We inspect the $m = 2$ orbital and the associated metastable condensate. The upper panels summarize the results of the classical stability analysis. Three classical measures are used to characterize the stability of the SP as a function of the interaction u . The first measure is γ_o , the largest positive imaginary part of the eigenvalues of the Bogoliubov matrix W [Eq. (32)]. It tells us whether we have DS or instability. Note that the three-site chain lacks a GPE-like stability regime, meaning that $u_c = 0$.

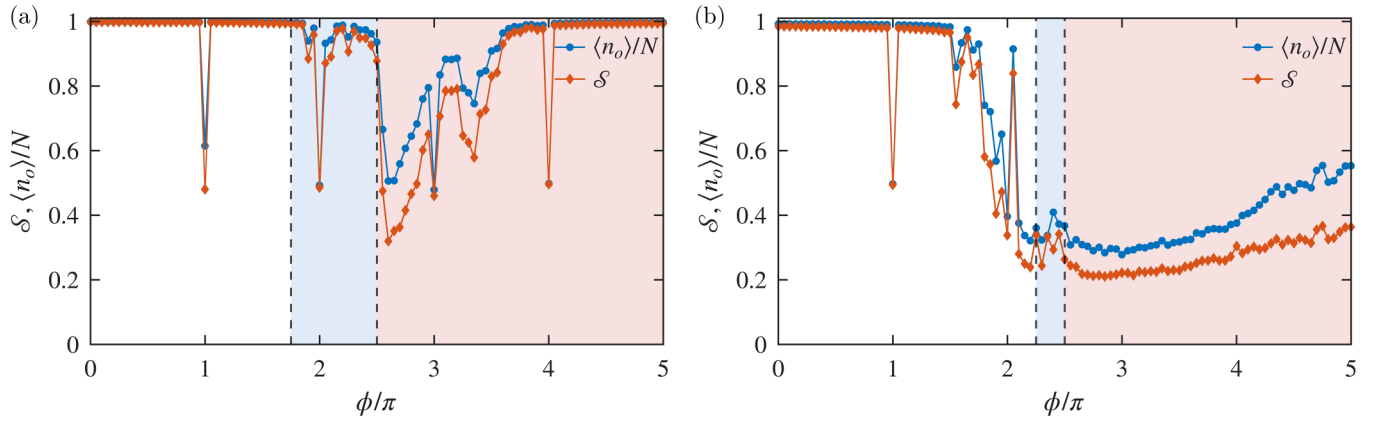


FIG. 13. Fingerprints of stability for a ring. We consider a five-site ring with $N = 30$ particles. The interaction is $u = 1$ (left) and $u = 4$ (right). We keep only the $P = 0$ eigenstates. The inspected orbital “o” is $m = 0$. The calculation of $\langle n_o \rangle_v$ and $\mathcal{S}$ is carried out for the “max” many-body eigenstate (see text). The plot shows the dependence of $n_{\max}$ and $\mathcal{S}_{\max}$ on ϕ , reflecting the level crossing at $\phi = \pi$ and the ES $\rightsquigarrow$ DS $\rightsquigarrow$ instability transitions that are indicated by dashed lines based on the Bogoliubov analysis of Fig. 1.

The two other measures, which are inspected in the upper panels of Fig. 14, are Lyapunov exponents. γ_{CS} is extracted from a trajectory that is launched in the chaotic sea, while γ_{SP} is the Lyapunov exponent of a trajectory that is launched in the vicinity of the SP. If the SP is unstable, and no stability island exists, one expects $\gamma_{\text{SP}} \sim \gamma_{\text{CS}}$, which is indeed what we

see. It is important to note that the Lyapunov exponent is not quantitatively correlated with γ_o ; notably, we might have weak or strong chaos irrespective of the stability of the unstable SP.

The second row of panels in Fig. 14 is based on the quantum tomography of the spectrum. It shows the dependence on u of $n_{\max}$ and $\mathcal{S}_{\max}$ and of an ergodicity measure σ that

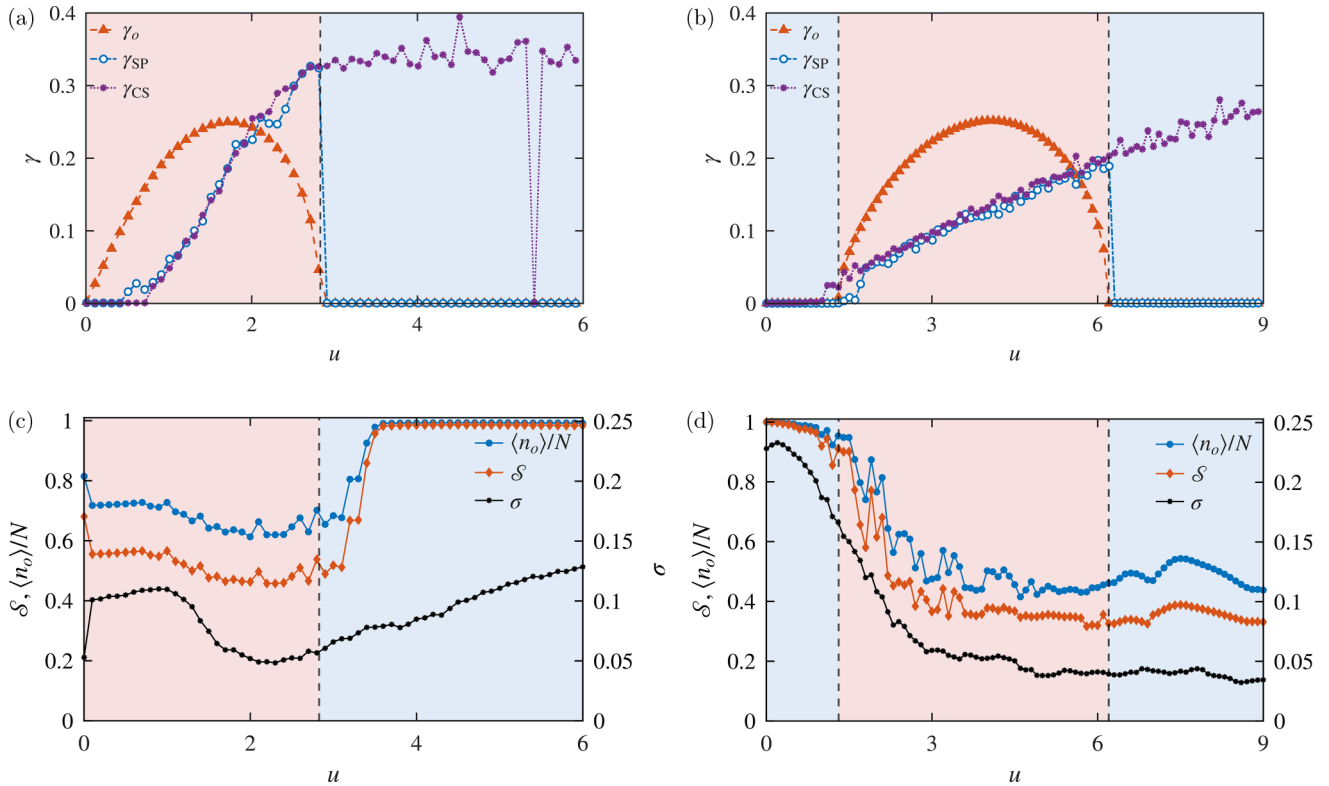


FIG. 14. Fingerprints of stability for a chain. We inspect the $m = 2$ orbital and the associated metastable condensate. Left and right panels are for three-site and five-site chains, respectively, featuring instability $\rightsquigarrow$ DS and DS $\rightsquigarrow$ instability $\rightsquigarrow$ DS transitions. In the quantum analysis, the number of particles is $N = 150, 20$, respectively, and we keep only the symmetric eigenstates. First row: Dependence of γ_o , γ_{SP} , γ_{CS} on u . Note that $\gamma_{\text{SP}} \sim 0$ if the SP is embedded in a quasiregular island, whereas ergodization leads to $\gamma_{\text{SP}} \sim \gamma_{\text{CS}}$. Second row: Dependence of $n_{\max}$ and $\mathcal{S}_{\max}$ and σ on u , where σ is the ergodicity measure defined in Eq. (43). The secondary instability $\rightsquigarrow$ DS transition for the five-site chain is barely reflected in the quantum case because the effective $\hbar \sim 1/N$ with $N = 20$ is rather large.

will be defined in the next section. One observes that the instability $\rightsquigarrow$ DS transition for the three-site chain and the DS $\rightsquigarrow$ instability transition for the five-site chain are well reflected. In contrast, the secondary instability $\rightsquigarrow$ DS transition for the five-site chain is barely reflected in the quantum case. This is hardly surprising, because the effective $\hbar \sim 1/N$ with $N = 20$ is rather large, and therefore the classical stability island is barely resolved as implied by Fig. 8.

C. Excitations

Speaking about “spectral signature,” the natural common inclination is to expect that there is a relation between many-body level spacings and the Bogoliubov frequencies. We have not emphasized this perspective because it has a rather limited validity in practice, and does not look useful or illuminating. Nevertheless, for completeness, we demonstrate this perspective.

On the basis of Bogoliubov’s diagonalization procedure, one expects to have the following approximation for eigenstates that reside in phase space in the vicinity of the SP:

$$E_v = E_{\text{SP}} + \sum_{v_q} v_q \omega_q. \quad (41)$$

Here, $v_q = 0, 1, 2, \dots$ are approximate quantum numbers and $v = \{v_q\}$ is regarded as a composite index. The sum $n_{\text{phonons}} = \sum_q v_q$ distinguishes between single-phonon excitations and multiphonon excitations. In Fig. 15(a), we display the expected spectrum, as a function of u , in the vicinity of the ground-state SP. The points are color coded according to n_{phonons} . In Fig. 15(b), we plot the many-body excitation energies based on the exact diagonalization. Here, the points are color coded as single-phonon or multiphonon excitations based on their spectral weight.

The *spectral weight* of an excitation is calculated as follows. We define the number-conserving Bogoliubov quasiparticle operator [77,78] as $C_q^\dagger = u_q A_q - v_q A_{-q}^\dagger$, where $A_q = \frac{1}{\sqrt{N}} \mathbf{a}_{k_0+q}^\dagger \mathbf{a}_{k_0}$, and the real coefficients (u_q, v_q) are determined via the diagonalization of $\mathbf{W}$. This operator is applied n_{phonons} times on the interacting ground state, hence generating synthetic multiphonon excitations. Then, each exact eigenstate is projected onto those synthetic excitations and color coded according to the dominant overlap. In particular, one-phonon excitations are colored in red, while states with $n_{\text{phonons}} > 3$ are color coded in gray.

Comparing panels (a) and (b) of Fig. 15, we see that, as expected, the Bogoliubov approximation provides a rather satisfactory approximation for the spectrum. Encouraged, we turn to apply the same procedure for the excitations in the vicinity of the energy E_{SP} of an excited condensate. The comparison shows that the usefulness of the Bogoliubov approximation is rather limited.

XIII. QUANTUM ERGODICITY

A superficial indication of ergodicity is narrow dispersion of the expectation value $\langle n_o \rangle$ within an energy window in the tomographic image of the spectrum. A more refined procedure is to look on the full distribution. Figure 16 displays the $P^v(n_o)$ of eigenstates that belong to a narrow window around the

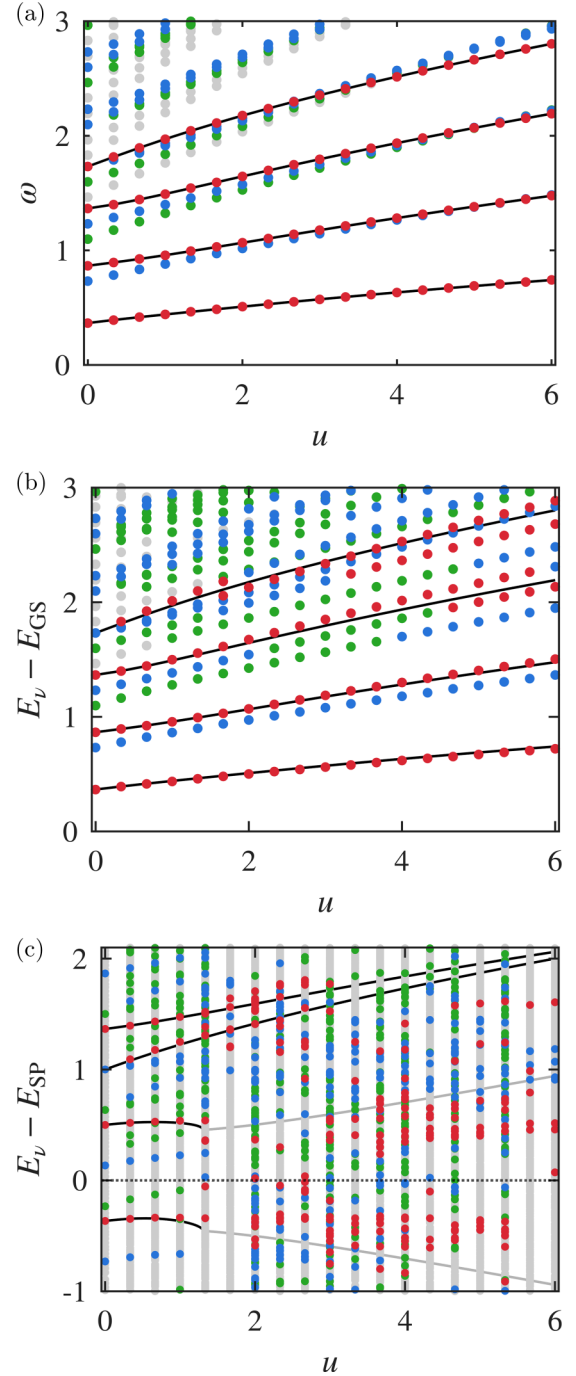


FIG. 15. Many-body excitation energies for a five-site chain. We consider the same chain of Fig. 12 with $N = 20$ particles. (a) Expected excitation spectrum based on Bogoliubov frequencies. Single-phonon excitations are in red, $n_{\text{phonons}} = 2, 3$ are in blue and green, while higher phonon occupations are shown in gray. (b) The exact excitation energies ($E_v - E_{\text{GS}}$) obtained through exact diagonalization. The n_{phonons} color code is determined as explained in the main text. (c) The same for the $m_o = 2$ condensate. The solid black lines represent the real Bogoliubov frequencies, while the gray lines represent the real part once they become complex.

energy E_{SP} of the inspected SP. The rows of each image are ordered by $\langle n_o \rangle$. An optional view on the same data is provided by Fig. 17, where the $P^v(n_o)$ plots are distinguished by color.

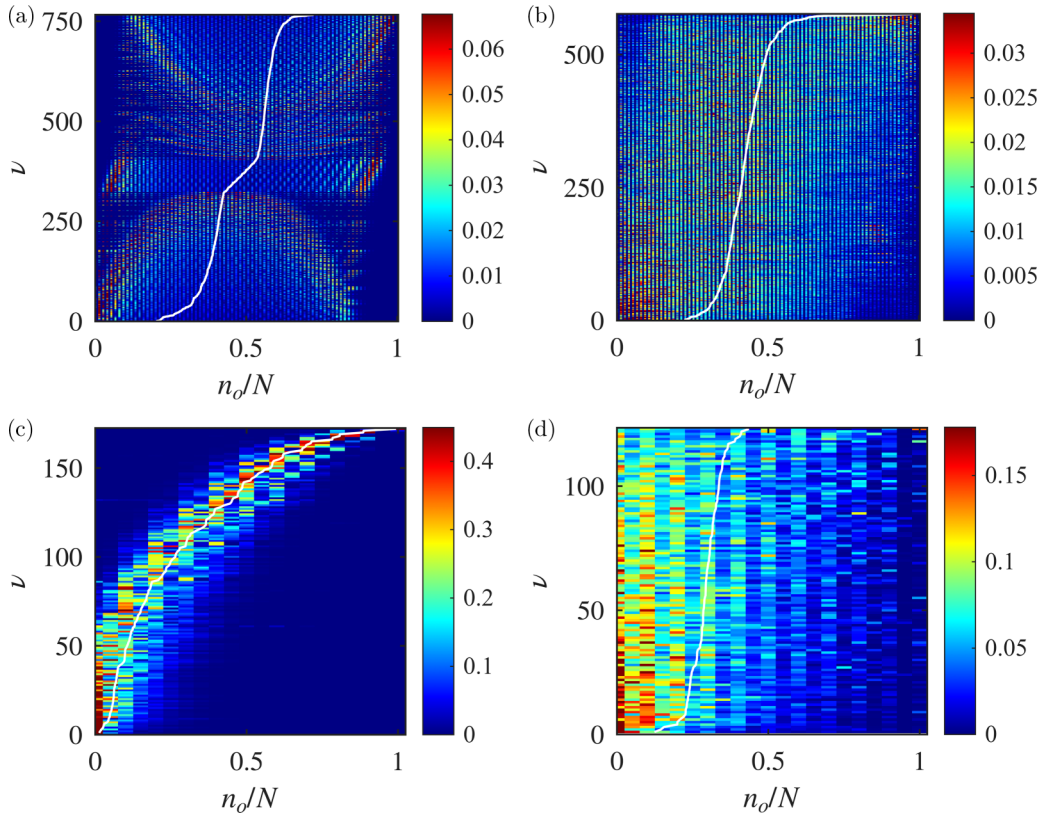


FIG. 16. Inspection of quantum ergodicity. Complementary to the tomography of Figs. 11 and 12. Each row of an image is a $P^\nu(n_o)$ distribution. These rows are ordered by $\langle n_o \rangle$. All the even-parity eigenstates within a narrow energy window around E_{SP} are included. The upper panels are for the three-site chain with $N = 150$. The lower panels are for the five-site chain with $N = 20$. Left and right panels are for $u = 0.5$ and $u = 3.5$, respectively.

In Fig. 17, we further compare the $P^\nu(n_o)$ of the individual eigenstates to the microcanonical distribution at the same energy, namely, $E \sim E_{\text{SP}}$. The quantum microcanonical distribution is

$$P^E(n_o) = \text{Average}_{\nu \in E}[P^\nu(n_o)], \quad (42)$$

where the average is taken over all the eigenstates within the energy window $[E, E + dE]$ that is narrow classically but contains a large number N_E of states. Namely, $\text{Average}_\mu[f_\mu] = (1/N_E) \sum_\mu f_\mu$. The corresponding classical distribution is obtained from long trajectories: Specifically, we inspect the distribution of the n_o coordinate over the simulation time. We see that there is, in general, a rather good agreement between the classical and the quantum $P^E(n_o)$ irrespective of ergodicity. A slight systematic deviation that is observed in the lower panels of Fig. 17 possibly reflects the difference between the Bose-Einstein and the Rayleigh-Jeans distribution [64].

In order to characterize quantum ergodicity within the energy window of interest, we calculate the dispersion

$$\sigma = \sqrt{\text{Average}_{\nu, n_o}[(P^\nu(n_o) - P^E(n_o))^2]}. \quad (43)$$

Here, the average is also over the initial value of the n_o coordinate. The results are displayed in Fig. 14 as a function of u . Small σ indicates that $P^\nu(n_o) \sim P^E(n_o)$ for most eigenstates. This is what we expect if the underlying phase space is fully chaotic. Large σ is possibly a signature for a structured

phase space that features remnants of quasi-integrable regions. Specifically, if we have stability island(s), we expect the eigenstates to be *localized* or possibly *hybrid*. The latter term implies that a quantum eigenstate can be a superposition of two localized pieces that have different phase-space locations. This is in the spirit of the chaos-assisted tunneling paradigm.

We turn to discuss details that are revealed by inspection of Fig. 16. For the $L_s = 5$ chain, the interpretation is rather simple. For small u , the phase space is quasi-integrable, and this is reflected in the ordering of the localized eigenstates. For larger u , chaos dominates, and all the eigenstates look similar (the residual systematic difference between them is an artifact of the ordering by $\langle n_o \rangle$).

We now turn to look on the $L_s = 3$ images of Fig. 16. For small u , we observe that the eigenstates are in general *hybrids*. If we hypothetically could turn off the hybridization, then we would find just two types of eigenstates: those that are localized in n_o and those that belong to the chaotic sea. Because of the hybridization, as an artifact of the row ordering, one might get the wrong impression that there are ~ 4 types of eigenstates. Looking in Fig. 14, we see that for small u , the fluctuations (σ) increase as a function of u . This reflects that hybridization is reduced. Namely, for small u , there are near-degeneracies in the spectrum that encourage hybridization, but as u is increased, these “resonances” are diminished due to level repulsion, and therefore the wavefunctions, *counterintuitively*, become less “ergodic.”

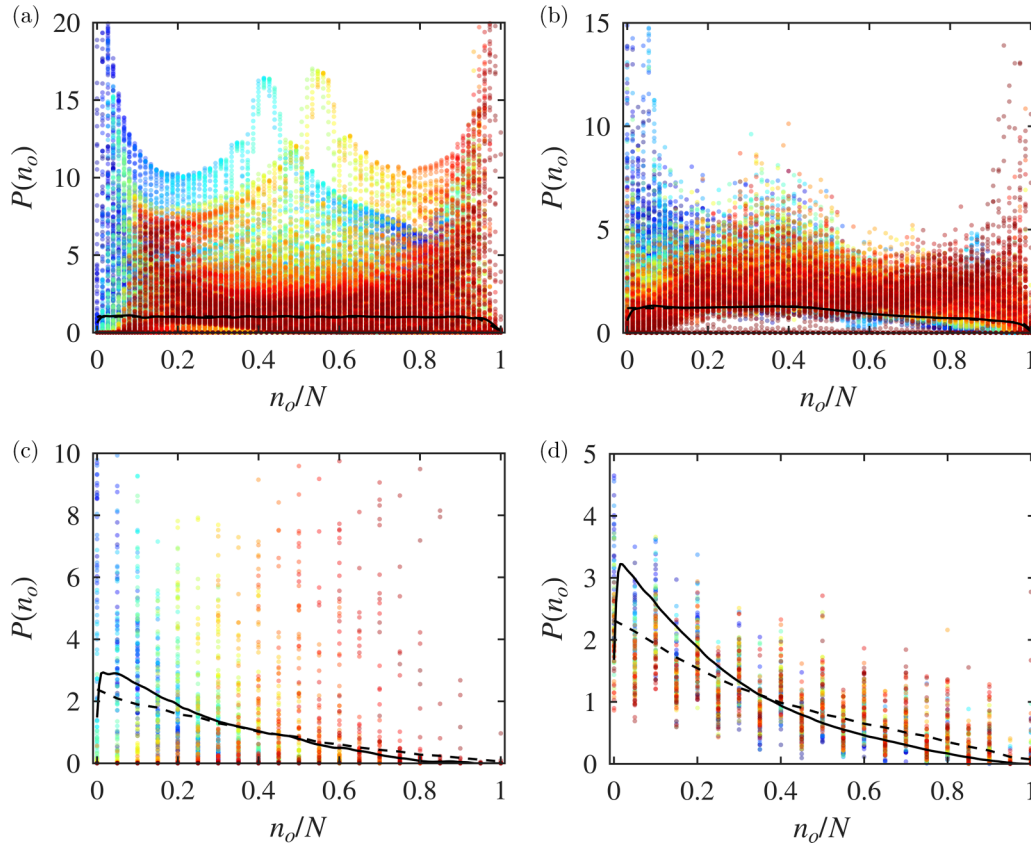


FIG. 17. Optional view over quantum ergodicity. The $P^v(n_o)$ of representative eigenstates (colored lines) are compared with the classical (solid) and quantum (dashed) microcanonical distributions (in the upper panels, the difference cannot be resolved). The dataset is the same as that of Fig. 16, and the panel arrangement is in one-to-one correspondence. The color code reflects $\langle n_o \rangle$ —It is used to distinguish the eigenstates.

Inspecting further the dependence of σ on u in the $L_s = 3$ case, as we enter the chaotic regime, the trend is reversed due to the induced ergodicity, and the fluctuations become smaller. Nevertheless, even when the chaotic sea dominates, there are still rather strong fluctuations, indicating remnants of quasiregular regions. For much larger values of u , the trend reverses again: Fluctuations become stronger as u increases. This reversed trend reflects the crossover to the DS regime, where the SP becomes stable.

XIV. SUMMARY

Systems that have two degrees of freedom, such as the Bose-Hubbard trimer, are in some sense special. We can say that they feature low-dimensional chaos: They have phase space with distinct quasiregular and chaotic regions. This is because the energy surface has $2d - 1 = 3$ dimensions, while the KAM barriers have $d = 2$ dimensions. For $d > 2$, the KAM barriers cannot divide the energy surface into distinct regions. Even if the nonlinearity is small, there is always slow leakage, also known as Arnold diffusion, via dynamical barriers.

Thus, in generic nonintegrable high-dimensional Hamiltonian systems, phase space is no longer partitioned by invariant barriers. Disregarding fragmentation due to energetic barriers, this facilitates transport across the whole energy surface

(connectivity). However, in practice, ergodicity is still limited by the possibly slow rate of exploration, by the persistence of sticky quasiregular structures, and by the associated wide distribution of dwell times.

Consequently, one may speculate that trimers are distinct compared to rings and chains with more sites. But as far as eigenstate tomography is concerned, the distinction between low- and high-dimensional chaos is blurred for complementary reasons: (1) In low-dimensional phase space, quantum dynamics allows leakage via dynamical barriers; (2) in high-dimensional phase space, quantum dynamics does not allow Arnold diffusion via small openings; and (3) quantum eigenstates might be hybrid.

The present work has considered *generic* Bose-Hubbard systems that have more than three sites. We have inspected the various transitions between regimes where the SP that supports condensation is ES, DS, or unstable. These transitions are quantified, as in Fig. 14, by both local Bogoliubov measures (notably γ_o) and by global Lyapunov measures (notably γ_{SP} and γ_{CS}). The inspected *quantum* measures are, respectively, those that detect metastable condensates ($n_{\max}$ and $\mathcal{S}_{\max}$) and the quantum ergodicity measure (σ).

For a ring, thanks to the interaction, the Bogoliubov frequencies of the supporting SP become positive, leading to ES. Chains, as opposed to rings, cannot support ES con-

condensates, but nevertheless, they are nonchaotic in the GPE limit, and can support DS condensates in the GPE-like interaction regime. Their Bogoliubov frequencies accumulate to zero as the GPE border is crossed. However, because the number of sites is finite, there is an additional DNLSE threshold u_c for the appearance of instability that can diminish the condensate. If L_s is too small, one might encounter $u_c = 0$ as opposed to the $u_c = \infty$ that characterizes the GPE limit.

The ES, DS, and instability regimes can be probed in state of the art cold-atom experiments. In a ring geometry [28–30], the transitions between these regimes are controlled by the Sagnac phase Φ , i.e., by the rotation frequency that is experimentally tunable. The signature of DS, as opposed to the ES, is the lack of thermodynamical stability, meaning that it is diminished by environmental decoherence. The survival of the superflow can be probed via time-of-flight imaging of the momentum distribution [28] (see, e.g., Fig. 15 there). For chains and for “box” confined condensates [31–36], the relevant control parameter is the interaction strength $u = NU/K$, which is tunable via a Feshbach resonance or the lattice depth. Recent experiments on far-from-equilibrium dynamics [37,38] provide motivation for further study of the relaxation dynamics.

In terms of methodology, our work has utilized an insightful semiclassical perspective (“tomography”) for dealing with a condensed matter many-body problem. Just by glancing at the tomographic image, e.g., Fig. 12, we can identify the underlying structure of phase space, to distinguish chaotic from quasiregular regions, and to detect metastable, hybrid, and self-trapped states. Our focus was on metastability versus ergodicity and how they depend on the number of sites. We emphasize the following: (1) Our approach is both numerically efficient and informative, as opposed to methods that are based on level statistics; and (2) our approach can be used for large rings, whereas the common practice in “quantum chaos” uses Poincaré sections whose visualization becomes challenging for more than two-degree-of-freedom systems. An exception that proves the rule is the visualization of classical structures and quantum states of four-dimensional maps as discussed by Richter *et al.* [79].

In the arena of high-dimensional chaos, one has to acknowledge the famous numerical experiment of Fermi-Pasta-Ulam and Tsingou (FPUT). The large L_s limit of a chaotic system can lead either to total microscopic chaos, as in the Boltzmann paradigm, or to integrability with diminished chaos, as in FPUT, which is also the case here in the GPE limit. Therefore, the clarification of the role of chaos for large rings is nontrivial. In the vast GPE/DNLSE literature, the role of chaos for finite L_s has not been sufficiently explored. Our emphasis was on the many-body quantum problem, highlighting the mixed nature of the dynamics. Accordingly, it is complementary to a recent work of the Freiburg group [43,44], which has explored the optimal route toward quantum chaos for the same Bose-Hubbard model. Their finding was that this is controlled by u . As opposed to that, our purpose was to detect signatures of mixed phase space, focusing on the manifestation of quasiregular islands that can support metastable condensates, whose stability is

controlled by the dimensionless parameters of Eqs. (10) and (11). We observe that with more degrees of freedom, such islands become better distinct from the ergodic sea, while their borders become ill-defined topologically. This stands in opposition to the very structured phase space of two-degree-of-freedom systems, as reflected in the tomographic quantum spectrum.

In some sense, the grand motivation for the present work is to provide tools and to achieve a better understanding regarding the validity or the failure of the semiclassical eigenfunction hypothesis of Percival. To the best of our understanding, while this hypothesis is widely accepted, a universal rigorous proof for all Hamiltonian systems does not exist. Rather, there are specific inquiries, mainly numerical. But alas, these inquiries usually refer to systems that have 2 dof, which we regard as nongeneric in this context, notably the well-studied Mushroom Billiard [80] and the Kicked Top [81]. An exception is Ref. [79] where the semiclassical eigenfunction hypothesis was studied and visualized for a 4D map. The failure of this hypothesis, even for relatively small systems, is likely to be of significance for studies of quantum thermalization and many-body localization, where the role of the underlying mixed phase space is ill understood. This holds, in particular, for strongly disordered systems, where thermalization can be modeled as the ergodization of small nearby chaotic subsystems that exchange particles and energy, sometimes referred to as hot spots [82].

ACKNOWLEDGMENT

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: BOGOLIUBOV ANALYSIS FOR LONG CHAINS

The lowest Bogoliubov frequencies of the $m_o = 2$ stationary solution are presented in Fig. 18 for chains that have up to 100 sites. In the first panel, we show the first two frequencies for $L_s = 7, 9, 11, 13, 15$. As u is increased, the DNLSE instability is pushed to larger u values, and the GPE regime is exposed, where the negative frequency approaches zero. In the second panel, we demonstrate that the results in the GPE regime scale very well for chains with more than 20 sites. In Fig. 3, we showed the Bogoliubov frequencies for the $m_o = 4$ stationary solution of a chain that has $L_s = 51$ sites. There, the results are compared with the outcome of a simple-minded approximation, which is further discussed below.

The $\mathbf{P}$ matrix is determined by the SP wavefunction. For example, for $L_s = 7$, and $m_o = 2$, we get for zero interaction Eq. (26). Consequently, in the orbital representation,

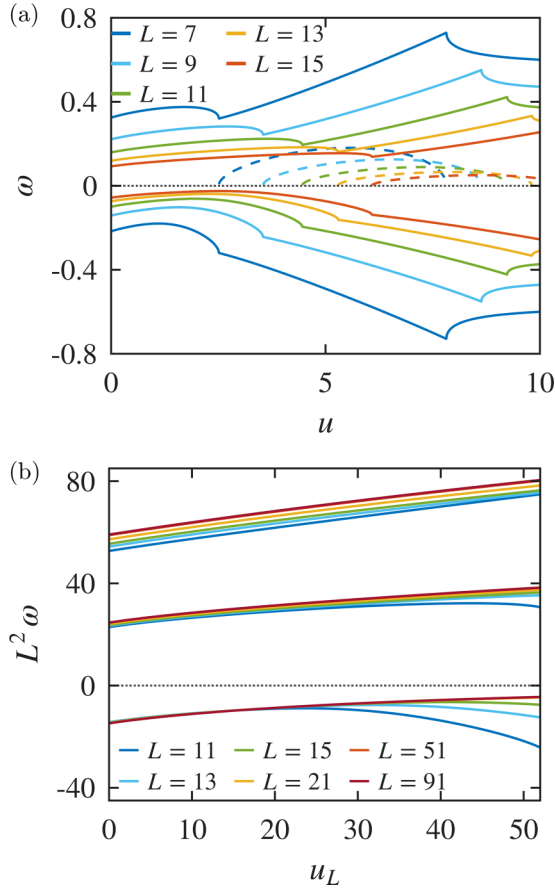


FIG. 18. Bogoliubov frequencies for short and long chains. The lowest Bogoliubov frequencies for the $m_o = 2$ stationary solution as a function of the interaction. The upper panel demonstrates how the complexity fades out for $L_s = 7, 9, 11, 13, 15$. The dashed lines are for $\text{Im}[\omega_q]$. The lower panel, with scaled axes Lu and $L^2\omega$, demonstrates convergence to the GPE limit, with $L_s = 11, 13, 15, 21, 51, 91$. Note that for more than 20 sites, the curves cannot be resolved.

we get

$$\tilde{\mathbf{P}}|_{u=0} = \frac{1}{16} \begin{pmatrix} 2 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 2 & 0 & 1 \\ 0 & -1 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & 2 \end{pmatrix}. \quad (\text{A1})$$

An additional example that illustrates the general case has been provided in Fig. 5 for the $m_o = 4$ stationary state of an $L_s = 51$ chain. As u is increased, the off-diagonal elements get smaller, but on the other hand, a pattern appears, as discussed in Sec. VII. On the basis of this observation, one may speculate that a leading order approximation for the eigenvalues of $\mathbf{W}$ can be obtained via diagonalization of either 2×2 blocks

(high levels) or 4×4 blocks (low levels):

$$\begin{pmatrix} \tilde{\mathcal{E}}_k & -\Delta_k \\ \Delta_k & -\varepsilon \end{pmatrix}, \quad (\text{A2})$$

$$\begin{pmatrix} \tilde{\mathcal{E}}_- & 2\Delta_q & -\Delta_k & -\Delta_q \\ 2\Delta_q & \tilde{\mathcal{E}}_+ & -\Delta_q & -\Delta_k \\ \Delta_k & \Delta_q & -\tilde{\mathcal{E}}_- & -2\Delta_q \\ \Delta_q & \Delta_k & -2\Delta_q & -\tilde{\mathcal{E}}_+ \end{pmatrix}, \quad (\text{A3})$$

where

$$\Delta_o = NU \sum_j \frac{2}{L} [\sin(k_o x_j)]^2 p_j, \quad (\text{A4})$$

$$\Delta_k = NU \sum_j \frac{2}{L} [\sin(k x_j)]^2 p_j, \quad (\text{A5})$$

$$\Delta_q = NU \sum_j \frac{2}{L} \sin((k_o + q)x_j) \sin((k_o - q)x_j) p_j, \quad (\text{A6})$$

$$\tilde{\mathcal{E}}_k = \varepsilon_k + 2\Delta_o - \mu = \varepsilon_k - \varepsilon_o(u) + 2\Delta_o - \Delta. \quad (\text{A7})$$

The $\tilde{\mathcal{E}}_{\pm}$ are the $\tilde{\mathcal{E}}_k$ for the two respective orbitals. For $u = 0$, one finds $\Delta_o = (3/2)\Delta$, while for $k \neq k_o$ it is $\Delta_k = \Delta$, and for $q \neq 0$ one finds $\Delta_q = (1/2)\Delta$. For large interaction, Δ_o approaches Δ , while Δ_q approaches 0 (see Fig. 5). The characteristic polynomial of the 4×4 block is a biquadratic equation $\lambda^4 - \alpha\lambda^2 + \beta = 0$, whose discriminant is positive if $\tilde{\mathcal{E}} > \Delta$, where $\tilde{\mathcal{E}} = (\tilde{\mathcal{E}}_+ + \tilde{\mathcal{E}}_-)/2$. Furthermore, in such a case, the roots come out real.

In practice, we see in Fig. 3 that the 2×2 blocks indeed provide a very good approximation for the high positive frequencies. But the 4×4 blocks provide only a quantitatively bad approximation for the low positive frequencies, and false instability instead of the negative frequencies. As discussed in the main text, this shortcoming should have been expected because the solitonic comb has been ignored.

APPENDIX B: BOGOLIUBOV FREQUENCIES, DERIVATION OF EXACT RESULTS

For a chain with an odd number of sites, the middle orbital, also known as the Dark state, is not affected by the interaction. For example, for a five-site chain, it is

$$\psi^{(3)} = \frac{1}{\sqrt{3}} \{1, 0, -1, 0, 1\}. \quad (\text{B1})$$

The Bogoliubov frequencies are indexed as $q = -2, -1, 0, 1, 2$, and we get

$$\omega_{+1} = [1/4 + u^2/18 + u/18\sqrt{u^2 - 9}]^{1/2}, \quad (\text{B2})$$

$$\omega_{-1} = -[1/4 + u^2/18 - u/18\sqrt{u^2 - 9}]^{1/2}, \quad (\text{B3})$$

$$\omega_{+2} = [3/4 + u^2/18 + u/18\sqrt{u^2 - 27}]^{1/2}, \quad (\text{B4})$$

$$\omega_{-2} = -[3/4 + u^2/18 - u/18\sqrt{u^2 - 27}]^{1/2}. \quad (\text{B5})$$

Also, the SP that supports the first excited condensate of the five-site chain is not affected by the interaction.

The nontrivial frequencies are the solution of a cubic equation

$$P(\lambda) = \lambda^3 - c_2\lambda^2 + c_1\lambda - c_0 = 0, \quad (\text{B6})$$

with coefficients

$$c_0 = \frac{1}{16} + \frac{u^3}{64}, \quad c_1 = \frac{3}{4} + \frac{u}{8} + \frac{u^3}{32}, \quad c_2 = \frac{9}{4} + \frac{u}{4} + \frac{u^2}{16}.$$

One defines

$$\Delta_0 = c_2^2 - 3c_1, \quad \Delta_1 = 2c_2^3 - 9c_1c_2 + 27c_0, \\ C = \left[\frac{1}{2}(\Delta_1 + \sqrt{\Delta_1^2 - 4\Delta_0^3}) \right]^{1/3}.$$

And then the roots [Eq. (34)] are obtained from Cardano's formula. For small u , the C comes out negative and consequently $|C|^2 = \Delta_0$, and the frequencies come out real. The critical value is the value of u for which the discriminant $\Delta_1^2 - 4\Delta_0^3$ becomes positive. It comes out $u_c \approx 1.307$.

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