Edge-state instabilities of bosons in a topological band

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In this work, we consider the dynamics of bosons in bands with non-trivial topological structure. In particular, we focus on the case where bosons are prepared in a higher-energy band and allowed to evolve. The Bogoliubov theory about the initial state can have a dynamical instability, and we show that it is possible to achieve the interesting situation where the topological edge modes are unstable while all bulk modes are stable. Thus, after the initial preparation, the edge modes will become rapidly populated. We illustrate this with the Su-Schrieffer-Heeger model which can be realized with a double-well optical lattice and is perhaps the simplest model with topological edge states. This work provides a direct physical consequence of topological bands whose properties are often not of immediate relevance for the near-equilibrium properties of bosonic systems.

I. INTRODUCTION

Bloch bands with non-trivial topological structure have been found to have important physical consequences for a variety of fermionic condensed matter systems including 1d conjugated polymers [1], quantum Hall systems [2], and topological insulators [3, 4]. Of central importance in each of these systems is the presence of topologically protected edge modes. There currently are growing efforts to create and understand bosons in non-trivial topological Bloch bands through the use of ultracold atomic systems in optical lattices [5–16]. One of the promising routes to such a realization is through the use of synthetic gauge fields [17, 18], and very recently a physical realization of the Hofstadter model has been achieved [19, 20]. However, the physical consequences of topologically non-trivial bands is less direct for the near-equilibrium properties of bosons than it is for fermions since bosons will generally populate the lowest energy single-particle states, while higher-energy topological edge states will be unoccupied. Experimental probes for edge states in such systems typically involve directly exciting bosons from the condensate into these modes (see, for instance, [21]).

In this work, we consider the evolution of a bosonic system (with topological edge modes) initially prepared in a higher energy band which has a dynamical instability. Dynamical instabilities, which give exponential growth of unstable modes in a conservative system, have received considerable experimental and theoretical attention with ultracold atoms (see, for instance, [22–28]). We show that it is possible to have the interesting situation where the edge modes are unstable while all of the bulk modes are stable. Therefore, after the system is allowed to evolve the bosons will rapidly (exponentially fast) occupy the edge modes. Apart from being an experimental probe of edge modes, the present work, more interestingly, proposes a new type of non-equilibrium dynamics where bosons under a dynamical instability rapidly populate these modes. While a 'holy grail' of current efforts with bosons in topological bands is to realize strongly-interacting fractional quantum Hall phases, the dynamics proposed here exists in the more common weakly-interacting regime.

II. BOGOLIUBOV-SSH HAMILTONIAN

Our work is partially inspired by the recent 'twin atomic beams' experiment [26]. In this experiment, bosons are initially prepared in the first excited transverse mode of a tube-shaped quasi one-dimensional trap and allowed to evolve. The system exhibits a dynamical instability and beams peaked at opposite momenta propagate longitudinally. We propose a variation of this set-up where the system is instead prepared in a quasi one-dimensional optical lattice potential which has single-particle states with non-trivial topology. For the non-interacting theory, we take the Su-Schrieffer-Heeger (SSH) Hamiltonian [1, 29]

$$\hat{\mathcal{H}}_0 = -J \sum_n \left[(1 + \bar{\epsilon}(-1)^n)(\hat{a}_n^\dagger \hat{a}_{n+1} + \text{H.c.}) - 2\hat{a}_n^\dagger \hat{a}_n \right] \tag{1}$$

which describes bosons hopping in a double-well 1d optical lattice [30]. In (1), $\bar{\epsilon}$ gives the magnitude of staggering in the hopping where $0 \leq \bar{\epsilon} \leq 1$, and we have included an overall shift in the chemical potential so that the lowest single-particle energy is zero. We choose to work with the SSH Hamiltonian (1) since it is perhaps the simplest model which possesses topological edge modes. However, the main results of this work are expected to hold for any system with edge modes. Measuring the Zak phase of the Rice-Mele model (which is the SSH model with staggering in the onsite energies) was the focus of a recent experimental work [12]). Methods of realizing fractionalized excitations of ultracold fermions in the SSH model were also proposed in [31, 32].

In [33], it was shown that adding an additional term to (1) with imaginary staggering in the on-site potential of the form $\hat{\mathcal{H}}' = i|\delta| \sum_n (-1)^n \hat{a}_n^\dagger \hat{a}_n$ can give exponential growth of the edge modes. Such a term will render

the full Hamiltonian non-hermitian, but can arise effectively for photons in waveguides. Here, we instead consider a fully hermitian Hamiltonian $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_1$ that arises naturally when performing a Bogoliubov expansion about the initial state of the aforementioned experiments where

$$\hat{\mathcal{H}}_1 = \sum_n \left[(u - \Delta)\hat{a}_n^\dagger \hat{a}_n + \frac{1}{2} u(\hat{a}_n \hat{a}_n + \text{H.c.}) \right] \quad (2)$$

contains the anomalous terms. In (2), $u = U n_0$ where U is the on-site Hubbard interaction and n_0 is the average number of particles per site for the initial state. The parameter Δ is related to the mean-field energy difference between the initial excited and ground state. That is, when $\Delta = 0$, one recovers the Bogoliubov theory of bosons condensed in the SSH lattice, and when $\Delta > 0$, there can be a dynamical instability. A derivation of this Hamiltonian is presented in the Appendix. We also point out that Hamiltonians of this form also arise in the context of quenched spinor condensates [34, 35], but here we will focus on scalar condensates prepared in a higher-energy band for definiteness.

III. GENERAL FORMALISM FOR QUADRATIC BOSONIC SYSTEMS

In the following, we will briefly describe the general methods used to compute the dynamical instabilities in finite systems. Considering a lattice with N sites, one can write the full Hamiltonian as $\hat{\mathcal{H}} = \frac{1}{2}\hat{\Psi}^\dagger H \hat{\Psi}$ where $\hat{\Psi} = (\hat{a}_1, \ldots, \hat{a}_N, \hat{a}_1^\dagger, \ldots, \hat{a}_N^\dagger)^T$ and the Bogoliubov de Gennes (BdG) Hamiltonian H is a $2N \times 2N$ Hermitian matrix which can be directly determined from (1) and (2). It is straightforward to see that the solution to the Heisenberg equations of motion $i\hbar \partial_t \hat{\Psi} = [\hat{\Psi}, \hat{\mathcal{H}}]$ is given by

$$\hat{\Psi}(t) = e^{-\frac{i}{\hbar}\tau_z H t}\hat{\Psi}(0). \quad (3)$$

Here, $\tau_\alpha = \sigma_\alpha \otimes \mathbb{1}$ where σ_α are Pauli matrices (where α can be x, y, or z) and $\mathbb{1}$ is the identity matrix. Since $\tau_z H$ is in general not Hermitian, it may have complex eigenvalues. When this occurs, the system is said to have a dynamical instability. This can be contrasted with the analogous problem of quadratic fermionic Hamiltonians which cannot have complex modes and therefore will never have a dynamical instability. To further understand (3), we consider the BdG equation

$$\tau_z H \psi_{i\pm} = \pm E_i \psi_{i\pm} \quad (4)$$

where $\psi_{i\pm}$ is a $2N$ dimensional eigenvector.

For our problem, as is verified numerically, the eigenvalues of $\tau_z H$ are either purely real or imaginary. We will consider these cases separately. Because of the symmetry $\tau_x H \tau_x = H^*$, the real eigenvalues occur in pairs $\pm E_i$ (as already indicated in (4)) with $\psi_{i-} = \tau_x \psi_{i+}^*$. For the real case, eigenvectors can be normalized as $\psi_{i+}^\dagger \tau_z \psi_{i'+} = \delta_{ii'}$,

$\psi_{i-}^\dagger \tau_z \psi_{i'-} = -\delta_{ii'}$, and we also have that $\psi_{i+}^\dagger \tau_z \psi_{i'-} = 0$ [36]. We now introduce the operators $\hat{\alpha}_i = \psi_{i+}^\dagger \tau_z \hat{\Psi}$ (or $\hat{\alpha}_i^\dagger = -\psi_{i,-}^\dagger \tau_z \hat{\Psi}$) which can be seen to satisfy bosonic commutation relations and diagonalize the stable portion of the full Hamiltonian.

We now consider the imaginary eigenvalues of $\tau_z H$. These will also occur in $\pm$ pairs since for a right eigenvector ψ_{i+} of energy E_i, we can obtain a left eigenvector $\psi_{i+}^\dagger \tau_z$ of energy $E_i^* = -E_i$. These eigenvectors can be normalized as $\psi_{i+}^\dagger \tau_z \psi_{i'-} = i\delta_{ii'}$ and we also have that $\psi_{i+}^\dagger \tau_z \psi_{i'+} = \psi_{i-}^\dagger \tau_z \psi_{i'-} = 0$ [36]. The operators defined as $\hat{x}_i = i\psi_{i-}^\dagger \tau_z \hat{\Psi}$ and $\hat{p}_i = -i\psi_{i+}^\dagger \tau_z \hat{\Psi}$ can then be seen to satisfy canonical commutation relations $[\hat{x}_i, \hat{p}_{i'}] = i\delta_{ii'}$. Equations can be simplified further by introducing the bosonic operators $\hat{\beta}_i = \frac{1}{\sqrt{2}}(e^{-i\frac{\pi}{4}}\hat{x}_i + e^{i\frac{\pi}{4}}\hat{p}_i)$. Then, together with the results from the real eigenvalues, we are able to rewrite the full Hamiltonian in the quasi-diagonal form

$$\hat{\mathcal{H}} = \sum_i (E_i + 1/2)\hat{\alpha}_i^\dagger \hat{\alpha}_i + \sum_i' \frac{1}{2}|E_i|(\hat{\beta}_i \hat{\beta}_i + \hat{\beta}_i^\dagger \hat{\beta}_i^\dagger) \quad (5)$$

where the first summation is over stable modes and the second (primed) summation is over unstable modes [37]. Note that a Hamiltonian that has a dynamical instability cannot be brought fully to diagonal form. It is straightforward to adapt the above formalism to the momentum basis or continuous systems, which will be done in the following paragraphs.

IV. BULK MODES

We will now focus on performing the above explicitly for our model. The bulk modes are expected to be well-approximated by applying periodic boundary conditions. It is easiest to begin by working in a basis which diagonalizes the non-interacting SSH Hamiltonian (1). It is straightforward to find that the non-interacting band energies are

$$\xi_k^{(1,2)} = 2J \mp 2J\sqrt{\cos^2(k) + \bar{\epsilon}^2 \sin^2(k)} \quad (6)$$

where k is restricted to the reduced Brillouin zone $[-\pi/2, \pi/2]$ (for simplicity we set the lattice constant to unity). These non-interacting bulk bands (6) satisfy $\xi_k^{(1)} \in [0, 2J(1-\bar{\epsilon})]$, $\xi_k^{(2)} \in [2J(1+\bar{\epsilon}), 4t]$. Writing (1,2) in this basis, one finds that the Bogoliubov energies are the eigenvalues of $\tau_z H_k$ where $H_k = (2J + u - \Delta)\mathbb{1} \otimes \mathbb{1} + \frac{1}{2}\left(\xi_k^{(2)} - \xi_k^{(1)}\right)\mathbb{1} \otimes \sigma_z + u\sigma_x \otimes \mathbb{1}$ ($\mathbb{1}$ here is the 2×2 identity matrix). Through this, the bulk energies are evaluated to be

$$E_k^{(n)} = \sqrt{(\xi_k^{(n)} - \Delta)(\xi_k^{(n)} - \Delta + 2u)}. \quad (7)$$

When $\Delta = 0$, (7) is real for all values of k and one recovers the phonon modes of bosons condensed in
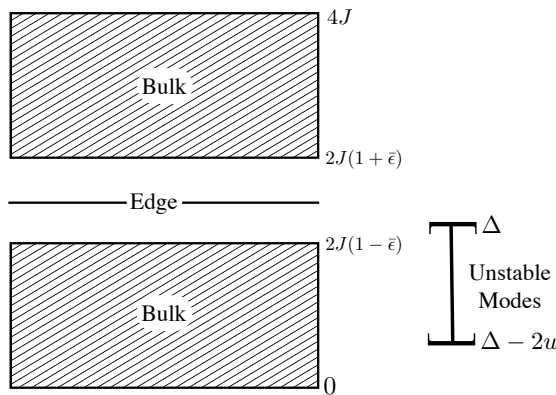
FIG. 1. Schematic description of dynamical instability. Left: energies of the *non-interacting* bulk and edge states. Right: region where dynamical instability occurs for a particular value of parameters. For the parameters illustrated in this figure, only the bulk modes in the lower band will be unstable.

the SSH lattice potential which has sound speed $c = \sqrt{2uJ(1-\bar{\epsilon}^2)}/\hbar$. On the other hand, when $\Delta > 0$, it is possible to have imaginary values of (7). In particular, a bulk mode that satisfies

$$\Delta - 2u < \xi_k^{(n)} < \Delta, \qquad (8)$$

will correspond to a dynamical instability. The condition for these modes to be stable/unstable is shown pictorially in Fig. 1.

V. EDGE MODES

We now move on to a description of the edge modes of our system. It is well known that the non-interacting SSH model can have topological mid-gap states localized at the edge of the system [1]. The existence of such states are predicted by the non-trivial Zak phase of the bulk banks of the SSH model [38]. More precisely, an edge mode of energy $2J$ will be present if a site at the boundary is connected with the smaller of the two hopping parameters, $J(1-|\bar{\epsilon}|)$ and $J(1+|\bar{\epsilon}|)$. We will restrict our attention to systems with an odd number of sites N, with the first site labelled by $n = 1$, thus ensuring precisely one edge mode in the non-interacting spectrum at the left-hand side of the system.

We now proceed to analyze the fate of the edge mode when the anomalous portion of the Hamiltonian (2) is accounted for. As a model for the edge mode, we allow $\bar{\epsilon}$ in (1) to depend on position and thus replace $\bar{\epsilon} \to \epsilon_n$. We take ϵ_n to have a localized "kink" so that $\epsilon_n \to \pm\bar{\epsilon}$ far to the right (left) of the kink. That is, moving across the kink changes the sign of ϵ_n. This lattice defect will bind a state which is topologically equivalent to an edge

mode [3, 39, 40]. We next decompose $\hat{a}_n$ as

$$\hat{a}_n = e^{i\frac{\pi}{2}n}\hat{b}_n + e^{-i\frac{\pi}{2}n}\hat{d}_n \qquad (9)$$

where the right and left movers, $\hat{b}_n$ and $\hat{d}_n$, are taken to be slowly varying on the scale of the lattice constant (we will drop second second and higher order derivatives in the continuum limit of these terms). This approximation is expected to be valid for small $\bar{\epsilon}$ since for this case, the edge mode is primarily composed of states at the band edges [1]. Inserting (9) into (1,2), taking the continuum limit $\hat{b}_n, \hat{d}_n \to \hat{b}(x), \hat{d}(x)$, and dropping higher derivatives, we find $\hat{\mathcal{H}} = \frac{1}{2}\int dx\hat{\Psi}^\dagger(x)H(x)\hat{\Psi}(x)$ where $\hat{\Psi}(x) = (\hat{b}(x), \hat{d}(x), \hat{b}^\dagger(x), \hat{d}^\dagger(x))^T$ and here the BdG Hamiltonian is

$$H = (2J + u - \Delta)\mathbb{1} \otimes \mathbb{1} + 2J(-i\partial_x)\sigma_z \otimes \sigma_z \qquad (10)$$
$$- 2J\epsilon(x)\sigma_z \otimes \sigma_y + u\sigma_x \otimes \sigma_x.$$

For simplicity, we choose the kink to be centered at $x = 0$ and therefore take $\epsilon(x)$ to be antisymmetric about this point. Since H only involves first order derivatives, the BdG equation for positive energy, $\tau_z H(x)\psi_+(x) = E\psi_+(x)$, has the general solution

$$\psi_+(x) = e^{\int_0^x dx' F(x')}\psi(0) \qquad (11)$$

where $F(x) = \frac{1}{2J}[iE\mathbb{1}\otimes\sigma_z - i(2J + u - \Delta)\sigma_z \otimes \sigma_z + 2J\epsilon(x)\mathbb{1}\otimes\sigma_x + iu\sigma_y \otimes \sigma_y]$.

We search for a solution (11) which exponentially decays away from the kink and thus require

$$F|_{\epsilon=\bar{\epsilon}}\,\psi_+(0) = -\kappa_1\psi_+(0) \qquad (12)$$
$$F|_{\epsilon=-\bar{\epsilon}}\,\psi_+(0) = \kappa_2\psi_+(0) \qquad (13)$$

for $\kappa_1, \kappa_2 > 0$. Subtracting (12) from (13) gives

$$2\bar{\epsilon}\,\mathbb{1}\otimes\sigma_x\,\psi_+(0) = -(\kappa_1 + \kappa_2)\psi_+(0). \qquad (14)$$

Therefore, $\psi_+(0) \propto \chi \otimes \chi_{-x}$ where $\sigma_x\chi_{-x} = -\chi_{-x}$ and χ is to be determined. Adding (12) and (13) with this condition on $\psi_+(0)$ then gives

$$iE\chi \otimes \chi_x - i(2J + u - \Delta)\sigma_z\chi \otimes \chi_x - u\,\sigma_y\chi \otimes \chi_x$$
$$= J(\kappa_2 - \kappa_1)\chi \otimes \chi_{-x} \qquad (15)$$

where $\sigma_x\chi_x = \chi_x$. This forces $\kappa_1 = \kappa_2 = \bar{\epsilon}$ and (15) is simplified to

$$[(2J + u - \Delta)\sigma_z - iu\sigma_y]\chi = E\chi. \qquad (16)$$

From this, the energy of the edge mode immediately follows:

$$E_{\text{edge}} = \sqrt{(2J - \Delta)(2J - \Delta + 2u)} \qquad (17)$$

which will be imaginary when

$$\Delta - 2u < 2J < \Delta. \qquad (18)$$

By comparing (8) and (18) one sees that for certain parameters, it is possible to have the situation where the edge mode is unstable but all bulk modes are stable. The optimal value of Δ for this to occur is $\Delta = \Delta_* \equiv 2J + u$ so that the region of unstable modes is centered in the gap (cf. Fig. 1). Then it is clear that all of the bulk modes will be stable if $u < 2J\bar{\epsilon}$. At the optimal value of Δ, we also have $E_{\text{edge}} = iu$ and the BdG wave function (11) can be found from (12,13) and takes on the relatively simple form

$$\psi_+(x) = \mathcal{N}e^{-\bar{\epsilon}|x|}(\omega, \omega^{-3}, \omega^{-1}, \omega^3)^T \qquad (19)$$

where $\omega = e^{i\frac{\pi}{4}}$ and $\mathcal{N}$ is a (real) normalization constant. The overall phase is chosen so that $\psi_+^*(x) = \tau_x \psi_+(x)$. A very similar analysis can be used to find $\psi_-(x)$.

We now consider the experimentally relevant case of starting with a vacuum state of $\hat{a}_n$ bosons. This occurs for the case when all atoms are prepared in the higher-energy band [26] (see also the Appendix). Quantum fluctuations will trigger the evolution of this state (which at the classical level is stationary) into the lower band. To elucidate this behavior, we consider the time dependence of the population per site in the lowest band given by

$$G_n(t) \equiv \langle \hat{a}_n^\dagger(t)\hat{a}_n(t) \rangle \qquad (20)$$

where $\hat{a}_n(t) = e^{\frac{i}{\hbar}\hat{\mathcal{H}}t}\hat{a}_n e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t}$ in the Heisenberg picture and the expectation value is evaluated with the vacuum state corresponding to zero initial population in the lower band. We take a finite system with an odd number of sites, so that the edge mode decays to the right from site $n = 1$ (note that we number the lattice sites so that $n > 0$). We consider the case where only the edge mode is unstable and take $\Delta = \Delta_*$, with $u < 2J\bar{\epsilon}$. The BdG wave function (19) can then be used to find an expression for the time-dependent population of the atoms in the lowest band at a particular site when $|\bar{\epsilon}| \ll 1$. Reverting back to the case of a discrete lattice, we find

$$G_n(t) = 4\bar{\epsilon}e^{-2\bar{\epsilon}n}\sin^2\left(\frac{\pi n}{2}\right)\sinh^2\left(\frac{ut}{\hbar}\right). \qquad (21)$$

In deriving (21) we have neglected the contribution from the stable bulk modes which have oscillatory time dependence, and whose relative contribution to (20) becomes small for $|E_{\text{edge}}|t/\hbar \gg 1$. Note that the initial vacuum state will generically have non-zero overlap with the bulk states of system. For these parameters, the bulk band with energy $E_k^{(1)}$ will be energetically unstable, but the corresponding modes will not grow since the total energy is conserved. Eq. (21) gives exponential growth of the edge mode. One should note, however, that when the number of depleted bosons $\sum_n G_n(t)$ is on the order of the total particle number, the Bogoliubov theory breaks down, and (21) is inapplicable.
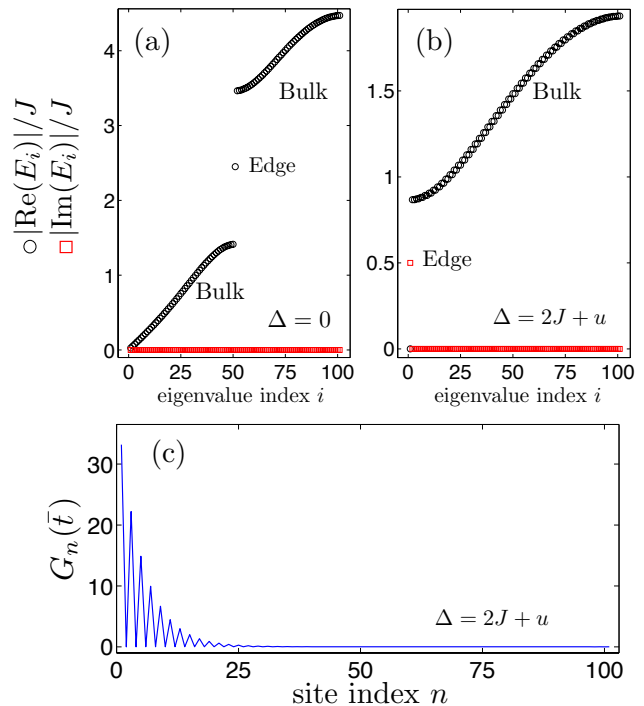

FIG. 2. (Color online) Top: the eigenvalues of $\tau_z H$ from direct diagonalization of (1,2) in ascending order for a lattice with $N = 101$ sites and parameters $u/J = \bar{\epsilon} = 1/2$. (a) has $\Delta = 0$ and so all modes are real while (b) has $\Delta = 2J + u$. (c): The population per site after time $\bar{t} = 30\hbar/J$ for $\Delta = 2J + u$. So that $G_n(\bar{t})$ extends over several lattice sites, the values $u/J = \bar{\epsilon} = 1/10$ were chosen in (c).

VI. NUMERICAL DIAGONALIZATION.

We now move on to discuss the direct numerical diagonalization of the $2N \times 2N$ BdG equation. This will allow us to validate the analytic results found previously, and also to access the regime where $\bar{\epsilon}$ is not small. Interestingly, the conditions established previously for the edge state to by stable/unstable remain accurate when $\bar{\epsilon}$ is not small. Results are shown in Fig. 2. Panel (a) shows the eigenvalues of the BdG equation for the case of $\Delta = 0$ which has all real eigenvalues, as expected. These are the Bogoliubov energies of bosons condensed in the ground state of the SSH model. In panel (b), the optimal value of $\Delta = \Delta_*$ is chosen. As is indicated by (8), (18) and confirmed by the diagonalization, the only imaginary eigenvalue is associated with the edge mode. The analytical expressions for the bulk and edge energies (7,21) show excellent agreement with the results from the numerical diagonalization. The population per site, $G_n(t)$, can be computed numerically from (3). In panel (c), $G_n(t)$ is plotted, again for the optimal value of Δ. For this panel, we set $\bar{\epsilon} = 1/10$ so that the edge mode extends across several lattice sites, but is still well-localized about the LHS of the system ($N = 101 > 1/2\bar{\epsilon}$). For the time shown

in the plot, the unstable edge has the dominant contribution to $G_n(t)$, and the expression (21) shows excellent agreement with the exact result shown in the figure.

VII. DISCUSSION AND CONCLUSION

The microscopic parameters entering (1, 2) for the proposed experiment of having an unstable edge mode but stable bulk modes are within current experimental range. The value of Δ can be tuned over a wide range of values by changing the trap confinement in the tight direction as discussed in the Appendix. Though the experiment in [26] is done without an optical lattice, their value of Δ is about a factor of four larger than the mean field interaction energy. Now consider tuning Δ to its optimal value, $\Delta = \Delta_* = 2J + u$, so that the region of unstable modes as pictured in Fig. 1 is centered in the gap. For non-zero u, the edge mode will have a dynamical instability. For all of the bulk modes to be (dynamically) stable, we have the further requirement $u < 2J\bar{\epsilon}$. This requirement is consistent with the initial state being in the superfluid regime (away from the Mott Insulator transition) and will occur when $\bar{\epsilon}$ is not too small.

Our treatment of finite systems with open boundary conditions is somewhat over-idealized in that experiments in ultracold gases normally also involve a confining potential $V(x_n)$ which adds the additional contribution $\hat{\mathcal{H}}_{\text{trap}} = \sum_n V(x_n)\hat{a}_n^\dagger \hat{a}_n$ to the full Hamiltonian. While a thorough treatment of the confining potential is beyond the scope of the present work, we note that it is shown in [41] that many of the features of edge modes remain when a harmonic confining potential is applied. Alternatively, it is possible to engineer sharp boundary conditions as described in [42] which are very similar to open boundary conditions. Finally, it may be possible to directly engineer a kink or domain wall using the recently developed methods to address single sites of an optical lattice [43, 44].

In summary, we have described a method through which the topological edge modes of a system can tuned to have a dynamical instability while all the bulk modes remain stable. This is particularly interesting since topological bands typically play an inessential role in condensed bosonic systems. To illustrate, motivated by its simplicity, we have considered the SSH model with anomalous terms. An interesting avenue of future study will be to consider similar preparations of two-dimensional Chern insulators [45]. A crucial difference with such systems is that the edge modes in the 2d systems have dispersion and so only a portion of them will be unstable. This work only concentrated on the quadratic theory expanded about the initial state, which will inevitably break down at sufficiently long times when the number of depleted bosons becomes comparable to the number of condensed bosons. Another interesting future direction is to use more elaborate theoretical techniques to explore such dynamics for longer times.

Appendix A: Derivation of the Bogoliubov-SSH Hamiltonian

In the following, we discuss a context in which the effective Hamiltonian given in Eqns. (1,2) of the manuscript arises. We consider a setup akin to that used in the experiment in [26], but in the presence of a double-well optical lattice. The full Hamiltonian of the system is

$$\hat{\mathcal{H}} = \int d^3r \left[\hat{\Phi}^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{trap}}(y,z) + V_{\text{lat}}(x) \right. \right.$$
$$\left. \left. -\mu \right) \hat{\Phi}(\mathbf{r}) + \frac{g}{2}\hat{\Phi}^\dagger(\mathbf{r})\hat{\Phi}^\dagger(\mathbf{r})\hat{\Phi}(\mathbf{r})\hat{\Phi}(\mathbf{r}) \right]. \quad \text{(A1)}$$

In this equation, $V_{\text{trap}}(y,z) = \frac{1}{2}m(\omega_y^2 y^2 + \omega_z^2 z^2)$ is a harmonic trapping potential, $V_{\text{lat}}(x)$ is the optical lattice potential, μ is the chemical potential, g is the interaction parameter related to the three-dimensional s-wave scattering length, and $\hat{\Phi}(\mathbf{r})$ are the bosonic field operators: $[\hat{\Phi}(\mathbf{r}), \hat{\Phi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')$. For $V_{\text{lat}}(x)$, we take a one-dimensional double-well lattice having, for instance, the form

$$V_{\text{lat}}(x) = V_1 \cos(Qx) + V_2 \cos(2Qx) \quad \text{(A2)}$$

with $V_1, V_2 > 0$. As in [26], we take tight confinement in the y and z directions with $\omega_y \lesssim \omega_z$ and consider an initial state that is in the first excited state of the trapping potential. We accordingly expand the bosonic field operator into the ground and excited bands (where the excited band corresponds to the first excited spatial mode of the trap): $\hat{\Phi}(\mathbf{r}) = \hat{\Phi}_g(\mathbf{r}) + \hat{\Phi}_e(\mathbf{r})$ where

$$\hat{\Phi}_g(\mathbf{r}) = \sum_n \phi_g(y,z)w_n(x)\hat{a}_{g,n} \quad \text{(A3)}$$

$$\hat{\Phi}_e(\mathbf{r}) = \sum_n \phi_e(y,z)w_n(x)\hat{a}_{e,n}. \quad \text{(A4)}$$

In this, the one-dimensional sum is over the lattice sites situated at the minima of $V_{\text{lat}}(x)$ in the x-direction. The Wannier orbital $w_n(x)$ is centered at site n, and $\phi_g(y,z)$ and $\phi_e(y,z)$ are ground and first excited spatial modes of the trap which are well approximated by harmonic oscillator wave functions for strong confinement. The orbitals $\phi_g(y,z)$ and $\phi_e(y,z)$ are taken to be real and are symmetrical under $z \to -z$, while $\phi_g(y,z) = \phi_g(-y,z)$ and $\phi_e(-y,z) = -\phi_e(y,z)$. Inserting $\hat{\Phi}(\mathbf{r}) = \hat{\Phi}_g(\mathbf{r}) +$

$\hat{\Phi}_e(\mathbf{r})$ into $\hat{\mathcal{H}}$, using the parity of $\phi_{e,g}$, and integrating over y and z, we obtain

$$\hat{\mathcal{H}} = \sum_n \Bigg[-J(1+\bar{\epsilon}(-1)^n)(\hat{a}_{g,n}^\dagger \hat{a}_{g,n+1} + \hat{a}_{e,n}^\dagger \hat{a}_{e,n+1} + \text{H.c.})$$
$$+ \frac{U_{gg}}{2}\hat{a}_{g,n}^\dagger \hat{a}_{g,n}^\dagger \hat{a}_{g,n}\hat{a}_{g,n} + \frac{U_{ee}}{2}\hat{a}_{e,n}^\dagger \hat{a}_{e,n}^\dagger \hat{a}_{e,n}\hat{a}_{e,n} \quad \text{(A5)}$$
$$+ 2U_{ge}\hat{a}_{g,n}^\dagger \hat{a}_{e,n}^\dagger \hat{a}_{g,n}\hat{a}_{e,n} + \frac{U_{ge}}{2}\hat{a}_{g,n}^\dagger \hat{a}_{g,n}^\dagger \hat{a}_{e,n}\hat{a}_{e,n}$$
$$+ \frac{U_{ge}}{2}\hat{a}_{e,n}^\dagger \hat{a}_{e,n}^\dagger \hat{a}_{g,n}\hat{a}_{g,n} - \tilde{\Delta}\hat{a}_{g,n}^\dagger \hat{a}_{g,n}$$
$$- \mu(\hat{a}_{g,n}^\dagger \hat{a}_{g,n} + \hat{a}_{e,n}^\dagger \hat{a}_{e,n}) \Bigg]$$

where $\tilde{\Delta} > 0$ is the energy difference between the ground and excited orbitals (in the limit of tight confinement, $\tilde{\Delta} = \hbar\omega_y$), and we have shifted the chemical potential. The nearest-neighbor hopping expressed as $-\int dx\, w_n^*(x)\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V_{\text{lat}}(x)\right)w_{n+1}(x)$ is $J(1+\bar{\epsilon})$ for n even and $J(1-\bar{\epsilon})$ for n odd (hopping further than nearest-neighbors is dropped). We also define $U_{\alpha\beta} = g\int d^3r\ \phi_\alpha^2(y,z)\phi_\beta^2(y,z)|w_n(x)|^4$. A similar analysis to the above is carried out in [46].

The Gross-Pitaevskii equation corresponding to (A5) will have the solution $a_{e,n} = \sqrt{(\mu+2t)/U_{ee}} \equiv \bar{a}_e$, $a_{g,n} = 0$ which corresponds to all bosons being in the excited band. Inserting $\hat{a}_{e,n} = \bar{a}_e + \delta\hat{a}_{e,n}$ into (A5) and expanding to quadratic order in $\delta\hat{a}_{e,n}$ and $\hat{a}_{g,n}$, we find (dropping the constant term)

$$\hat{\mathcal{H}}_{\text{B}} = \hat{\mathcal{H}}_g + \hat{\mathcal{H}}_e \quad \text{(A6)}$$

where

$$\hat{\mathcal{H}}_g = \sum_n \Bigg[-J(1+\bar{\epsilon}(-1)^n)(\hat{a}_{g,n}^\dagger \hat{a}_{g,n+1} + \text{H.c.}) \quad \text{(A7)}$$
$$+ (2J + U_{ge}n_0 - \Delta)\hat{a}_{g,n}^\dagger \hat{a}_{g,n} + \frac{U_{ge}n_0}{2}(\hat{a}_{g,n}\hat{a}_{g,n} + \text{H.c.}) \Bigg]$$

and

$$\hat{\mathcal{H}}_e = \sum_n \Bigg[-J(1+\bar{\epsilon}(-1)^n)(\delta\hat{a}_{e,n}^\dagger \delta\hat{a}_{e,n+1} + \text{H.c.}) \quad \text{(A8)}$$
$$+ (2J + U_{ee}n_0)\delta\hat{a}_{e,n}^\dagger \delta\hat{a}_{e,n} + \frac{U_{ee}n_0}{2}(\delta\hat{a}_{e,n}\delta\hat{a}_{e,n} + \text{H.c.}) \Bigg] .$$

In these equations, we have introduced $n_0 \equiv |\bar{a}_e|^2$ and $\Delta \equiv \tilde{\Delta} + U_{ee}n_0 - U_{ge}n_0$. Interestingly, at the quadratic level the dynamics of bosons in the ground and excited band is decoupled. It is straightforward to diagonalize $\hat{\mathcal{H}}_e$ and see that it is stable. Furthermore, retaining higher-energy bands will yield additional stable and gapped modes which are unimportant. The Hamiltonian $\hat{\mathcal{H}}_g$ is analyzed in the manuscript where the subscript g is dropped and $U \equiv U_{ge}$.

Appendix B: Evolution from the excited band

We now consider the evolution of the initial state where all atoms are in the excited band: $\langle\hat{a}_{g,n}\rangle = 0$, $\langle\hat{a}_{e,n}\rangle = \sqrt{n_0}$. Since this initial state is a solution of the Gross Pitaevskii equation, it will be stationary at the classical level. Quantum fluctuations, which are contained in (A6), will trigger the evolution. The atom number per site as a function of time is given by

$$F_n(t) = \langle\psi(t)|(\hat{a}_{g,n}^\dagger \hat{a}_{g,n} + \hat{a}_{g,e}^\dagger \hat{a}_{g,e})|\psi(t)\rangle \quad \text{(B1)}$$
$$= n_0 + \langle\psi(t)|\hat{a}_{g,n}^\dagger \hat{a}_{g,n}|\psi(t)\rangle + \langle\psi(t)|\delta\hat{a}_{e,n}^\dagger \delta\hat{a}_{e,n}|\psi(t)\rangle$$

where $|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{\mathcal{H}}_{\text{B}}t}|0\rangle$ and $|0\rangle$ is the vacuum state of $\hat{a}_{g,n}$ and $\delta\hat{a}_{e,n}$ bosons. This expression is valid when

$$\sum_n \langle\psi(t)|(\hat{a}_{g,n}^\dagger \hat{a}_{g,n} + \delta\hat{a}_{e,n}^\dagger \delta\hat{a}_{e,n})|\psi(t)\rangle \ll n_0 N. \quad \text{(B2)}$$

If there is a dynamical instability, there will inevitably be a time at which (B2) breaks down, but (B1) will be valid before then. In the manuscript, we investigate the behavior of $G_n(t) = \langle\psi(t)|\hat{a}_{g,n}^\dagger \hat{a}_{g,n}|\psi(t)\rangle$ which has exponential growth for a dynamical instability.

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