Letter

Topological properties of single-particle states decaying into a continuum due to interaction

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We investigate how topological Chern numbers can be defined when single-particle states hybridize with continua. We do so exemplarily in a bosonic Haldane model at zero temperature with an additional on-site decay of one boson into two and the conjugate fusion of two bosons into one. Restricting the Hilbert space to two bosons at maximum, the exact self-energy is accessible. We use the bilinear Hamiltonian H_0 corrected by the self-energy Σ to compute Chern numbers by two different approaches. The results are gauged against a full many-body calculation in the Hilbert space where possible. We establish numerically and analytically that the effective Hamiltonian $H_{\text{eff}} = H_0(\vec{k}) + \Sigma(\omega, \vec{k})$ reproduces the correct many-body topology if the considered band does not overlap with the continuum. In case of overlaps, one can extend the definition of the Chern number to the non-Hermitian H_{eff} and there is evidence that the Chern number changes at exceptional points. But the bulk-boundary correspondence appears to be no longer valid and edge modes delocalize.

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Introduction. The first striking topological effect discovered in condensed-matter physics is the integer quantum Hall effect [1]. Here the number of contributing edge modes defines the Hall conductivity [2,3] to an incredible precision revolutionizing metrology [4]. No nonlinearities occur [5,6]. Also, fractional charges are possible enabling the fractional quantum Hall effect [7]. Both topological effects gained their discoverers Nobel Prizes [8,9] and topology in condensed matter has continued to gain great interest in the last decades [10]. The possible types of topological order have been classified for Gaussian fermionic systems, both in the case of nonspatial and spatial symmetries [11–16]. A nontrivial topological ground state of a fermionic insulator cannot be connected adiabatically to the atomic limit without closing the gap or, if present, breaking the symmetry protecting the topological order. These topological states thus have nontrivial entanglement and typically also robust edge states [17–21]. For quantum Hall systems, in particular, topologically nontrivial ground states were proposed even for models without external magnetic field [22] and realized in experiment [23–26]. Numerous technological applications are expected not only in fermionic systems [27–30] but also in insulating quantum magnets, see, e.g., Ref. [31].

A crucial aspect of quantum Hall systems breaking time-reversal symmetry is the occurrence of robust, chiral edge modes which generically allow for motion only in one direction. These systems promise a high degree of tunability [32,33]. The difference between chiral edge modes propagating to the right and to the left is linked to the Chern number of a dispersive band, i.e., a topological invariant given by the Berry phase of a quantum state tracked around the Brillouin zone (BZ). This is commonly referred to as the bulk-boundary correspondence [34,35]. However, already for noninteracting systems, this correspondence must be used with caution because it only holds if the dispersive band is protected by *indirect* energy gaps [36,37]. Otherwise, the potential boundary mode is not localized but extends into the continuum. Such a breakdown of the bulk-boundary correspondence can also occur in manifestly non-Hermitian systems [38–42].

Thus, the hybridization of modes with continua can destroy the desired topological properties. Clearly, if a single-particle excitation is no longer defined in the whole BZ, then its Berry connection [43] cannot be defined in the standard way. Such a hybridization of single-particle states with continua is generic in interacting systems. Hence, a generalization of topological invariants is required. For ground states of fermionic topological insulators, topological invariants such as the Chern number can be expressed in terms of Green's functions at zero frequency [44–46]. Clearly, this allows for a straightforward extension to systems with interactions although zeroes in the Green's function need to be considered carefully. The appearance of edge modes at zero energy at the boundary between two topologically distinct phases is then the generic scenario, supporting the bulk-boundary correspondence. Similarly, a classification of symmetry-protected topological phases in interacting bosonic systems based on group cohomology theory exists [47].

Here we do not focus on the ground state and its topological properties but rather on the bands of elementary, single-particle excitations. Without interactions, the Berry

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curvature is unambiguously defined. Including interactions, two situations need to be distinguished: (i) If the single-particle states are adiabatically connected to the ones in the absence of interactions, i.e., the hybridization only renormalizes the single-particle states, then the Chern number can be defined in a mathematically rigorous way and the bulk-boundary correspondence holds if the edge mode is protected by an energy gap. (ii) If the single-particle states hybridize strongly with the continua, so that they merge with them, then a Chern number can be defined for the non-Hermitian effective Hamiltonian but not for the full Hamiltonian. The bulk-boundary correspondence appears not to be valid in this case.

We define a bosonic model reduced to the essentials which allows for various approaches to treat it. Our study provides evidence that the self-consistent solution of the effective single-particle problem defined by the noninteracting Hamiltonian plus the proper self-energy is the appropriate generalization to calculate Chern numbers in the interacting case. This approach provides a connection between many-particle Hermitian models and single-particle non-Hermitian models. We emphasize, however, that usually non-Hermiticity is invoked on the basis of gains and losses. Here, in contrast, we investigate a Hermitian many-body problem which can be reduced to an effective single-particle problem if the complex self-energy with its full frequency dependence is known. This effective problem can be non-Hermitian, but its non-Hermiticity depends on frequency.

Model. We consider interacting bosons on a honeycomb lattice with sublattices A and B described by

$$H = H_0 + H_{\rm int} \tag{1a}$$

$$H_0 = t_1 \sum_{\langle i,j\rangle} (b_i^\dagger b_j + \text{H.c.}) + t_2 \sum_{\langle\langle i,j\rangle\rangle} (e^{i\nu_{ij}\phi} b_i^\dagger b_j + \text{H.c.}) + M \sum_i \varepsilon_i b_i^\dagger b_i + E_0 \sum_i b_i^\dagger b_i \tag{1b}$$

$$H_{\rm int} = g \sum_i (b_i^\dagger b_i^\dagger b_i + \text{H.c.}), \tag{1c}$$

where b_i and $b_i^\dagger$ are bosonic annihilation and creation operators, respectively. The positive prefactors t_1, t_2, g, E_0, and M are energies, and $\nu_{ij} = +1$ if hopping from i to j is clockwise in a hexagon and $\nu_{ij} = -1$ otherwise. The local sign is $\varepsilon_i = 1$ if $i \in A$ and $\varepsilon_i = -1$ if $i \in B$. The sums over $\langle i, j\rangle$ and $\langle\langle i, j\rangle\rangle$ run over nearest neighbors and next-nearest neighbors, respectively. This bilinear part is analogous to the fermionic Haldane model which displays well-established topological properties with finite Chern numbers [22]. The on-site energy E_0 serves two purposes: First, E_0 needs to be sufficiently large so that the bosonic excitation energies are positive. Then, the ground state is the topologically trivial bosonic vacuum. Our focus is on the topological properties of the excited bands. Second, tuning E_0 and g allows us to control the strength of the hybridization between one-boson and two-boson states.

The cubic interaction $H_{\rm int}$ describes the decay of one boson into two bosons on the same site with coupling constant g or the inverse process, i.e., the fusion of two bosons into one. Terms of this kind occur generically in quantum magnets for spin waves in case of noncollinear order [48–50] as well as for triplons in valence bond solids [50–53]. We stress that one should first perform a Bogoliubov transformation to diagonalize the bilinear part including terms of two annihilation or creation operators. Otherwise, it is unavoidable to generalize the operator scalar product to a symplectic or paraunitary one, see for instance Refs. [36,54,55]. The diagonalized Hamiltonian is similar to (1) except that the hopping terms and the interaction terms have a certain spatial range. In this sense, H is an idealization adopted here not to be distracted by a plethora of parameters. We consider the cubic interaction because the continuum to which the single-particle states are coupled is then governed by only one free momentum while the relevant continuum for the quartic interaction requires two free momenta. Thus, the treatment of cubic terms is considerably easier than the one of quartic terms. The possibility of having cubic interactions is also a reason to consider a bosonic instead of a fermionic model where cubic terms do not occur in standard systems.

In order to deal with an exactly solvable limit, we restrict the Hilbert space to $\mathcal{H} = \mathcal{H}(0) \oplus \mathcal{H}(1) \oplus \mathcal{H}(2)$, where $\mathcal{H}(n)$ is the Hilbert space of exactly n bosons. Hence, the restriction allows for two bosons at maximum. Then, we can exactly determine the self-energy at zero temperature, see the Supplemental Material [56]. The efficient evaluation on meshes in the BZ of moderate sizes is carried out by means of a generalized continued fraction expansion derived in the Supplemental Material [56] based on mathematical tools described in Refs. [57–60]. Alternatively, we can consider the self-energy as the leading contribution in perturbation theory of quadratic order in g. In this view, the Hilbert space does not need to be restricted.

Chern numbers. For noninteracting systems, the Chern number of the n-th band is defined as $C = \frac{1}{2\pi}\int_{\rm BZ} F_{12} d^2k$, where $F_{12} = \partial_1 A_2 - \partial_2 A_1$ denotes the Berry curvature and $A_i(\vec{k}) = \langle u_n(\vec{k})|\partial_i|u_n(\vec{k})\rangle$ is the Berry connection. The states $|u_n(\vec{k})\rangle$ are the single-particle states at wave vector $\vec{k}$. In order to calculate these states, the coefficient matrix $H_0(\vec{k})$ of the bilinear Hamiltonian at this wave vector is sufficient. For the model under study, this amounts to the solution of a 2×2 problem at each given point of a mesh in the BZ. In our calculations, we use meshes ranging from 20×20 to 30×30. These sizes are sufficient to compute the Chern numbers [61].

For the interacting system, we proceed in three distinct ways:

Topological approach. We use the eigenstates of

$$H_{\rm top}(\vec{k}) = H_0(\vec{k}) + \Sigma(\omega = 0, \vec{k}) \tag{2a}$$

fulfilling

$$H_{\rm top}(\vec{k})|u_n(\vec{k})\rangle = E_n(\vec{k})|u_n(\vec{k})\rangle. \tag{2b}$$

Obviously, this is still a 2×2 problem for each $\vec{k}$. At zero frequency, the self-energy is Hermitian so that no issues from non-Hermiticity arise; $E_n(\vec{k})$ is real. Wang *et al.* showed that for fermionic models at $T = 0$ the sum $\sum_{\alpha\ \rm occ.} C_\alpha$ of the Chern numbers C_α obtained from $H_{\rm top}(\vec{k})$ for the occupied bands provides the Chern number of the ground state which defines the Hall conductivity [45,62].

Effective approach. We use the eigenstates of

$$H_{\text{eff}}(\omega, \vec{k}) = H_0(\vec{k}) + \Sigma(\omega, \vec{k}) \tag{3a}$$

fulfilling the self-consistent eigenvalue equation

$$H_{\text{eff}}(E, \vec{k})|u(E, \vec{k})\rangle = E(\vec{k})|u(E, \vec{k})\rangle. \tag{3b}$$

This is still a 2×2 problem for each $\vec{k}$ but with the calculation of the self-consistent $E(\vec{k})$ as additional challenge. For non-Hermitian diagonalizations, the right and left eigenstates differ, but they define fiber bundles over the manifold given by the torus of the BZ, allowing for the definition of quantized Chern numbers and it has been shown that they yield the same Chern numbers [38]. In Ref. [63], the suitability of the effective Hamiltonian $H_{\text{eff}}(\omega, \vec{k})$ was critically discussed because it did not provide the correct Chern number of fermionic ground states. Since, however, our focus is a different one it is worthwhile considering $H_{\text{eff}}(E, \vec{k})$.

Two-body approach. We use the eigenstates at a given total wave vector $\vec{k}$ in the total Hilbert space $\mathcal{H}$

$$H(\vec{k})|u_n(\vec{k})\rangle = E_n(\vec{k})|u_n(\vec{k})\rangle. \tag{4}$$

This is a standard Hermitian diagonalization problem, but in a large Hilbert space of which the dimension at fixed wave vector $\vec{k}$ is given by the number of sites in the model. Numerically, we deal with sizes of 100 to 1000 sites. The calculation of Berry connections does not pose a conceptual difficulty in the total Hilbert space as long as one can uniquely identify the relevant eigenstates. This is the crucial obstacle in the case of bands overlapping with the continuum.

Phase transition at gap closure. In a two-band system, the Chern number of a band does not change if it is only adiabatically modified while staying separated from the other band by a finite gap. Thus, a phase transition between regions of different Chern numbers must be accompanied by the vanishing of the direct energy gap between the two bands, i.e., at some $\vec{k}$,

$$\Delta E(\vec{k}) = |E_1(\vec{k}) - E_2(\vec{k})| = 0. \tag{5}$$

In the Haldane model, the gap closes for the chosen parameters $t_1 = t_2 = 1, \phi = \pi/2$ at the K point if $M = 3\sqrt{3}$. We vary M keeping the other parameters fixed and determine M_C where the gap closes. Then, we determine the Chern number in the regions $M < M_C$ and $M > M_C$.

Edge states. To assess the implications of nontrivial Chern numbers in the interacting case and hence the validity of the bulk-boundary correspondence, we calculate the inverse participation ratio (IPR) [64,65] on a honeycomb ribbon periodic in x direction with length N_x and finite width N_y in y direction with open boundary conditions, for details see Supplemental Material [56]. If the n-th eigenstate is localized, then the IPR stays finite $\lim_{N_y \to \infty} I_n = \text{const}$ while it vanishes $\lim_{N_y \to \infty} I_n \sim 1/N_y^{\alpha} \to 0$ with $\alpha > 0$ for a delocalized state [36] allowing us to determine whether or not a state is localized. Further evidence for (de) localization is obtained from the local density of states (LDOS), also provided in the Supplemental Material [56].

Case I: No overlap with the lower band. For large $E_0 = 28$ the bands do not overlap with the two-boson continuum, see Fig. 1(a). Figure 1(b) shows the dependence of M_C on the

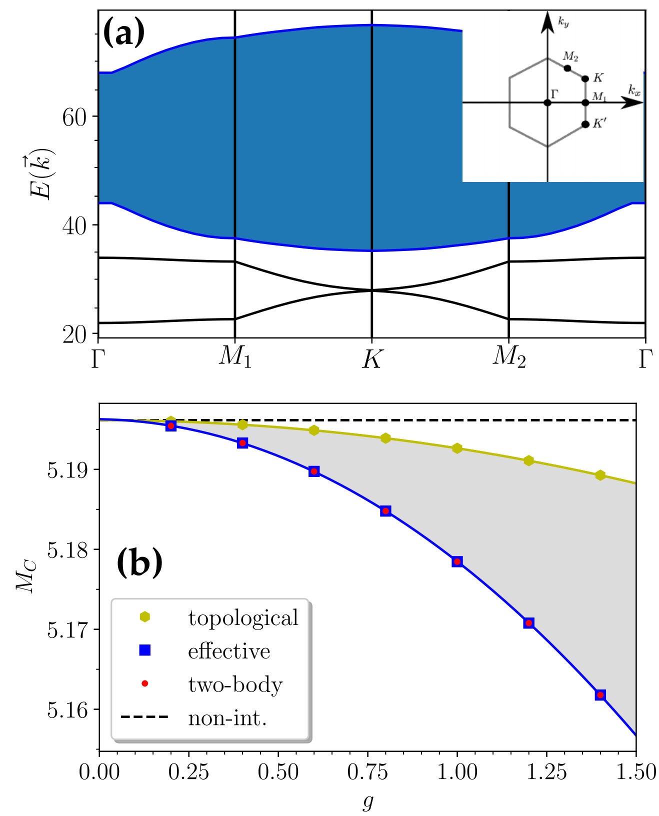

FIG. 1. (a) Two-boson continuum (colored) and renormalized single-boson bands for $E_0 = 28, M = 5.2$, and $g = 1.4$. (b) Critical values of M_C where the gap between the single-particle bands closes in the three approaches. Lines are quadratic fits.

coupling g. The effect is small because the system is in the perturbative regime where we estimate the self-energy to be $|\Sigma_{ij}| \approx \frac{g^2}{E_0} = 0.07$ for $g = 1.4$ and $E_0 = 28$. Within numerical accuracy, we find that the gap closure occurs at the K point in the BZ in all three approaches. We find $\Sigma(\omega, \vec{k})^\dagger = \Sigma(\omega, \vec{k})$ if $\omega < E^{(2)}_{\text{min}}(\vec{k}) = \min_{\alpha,\beta,\vec{q}}(E_\alpha(\vec{k} + \vec{q}) + E_\beta(-\vec{q}))$. Thus, we expect and observe only a (weak) renormalization of the noninteracting bands and an infinite lifetime of the excitations.

Due to the absence of overlap between the one-boson bands and the continuum, the Chern numbers are well defined in all three approaches. We find that $C_{\text{top}} = C_{\text{eff}} = C_{\text{2body}} = 1$ below the gray shaded area in Fig. 1(b), while $C_{\text{top}} = C_{\text{eff}} = C_{\text{2body}} = 0$ above. However, the approaches differ within the shaded area where $C_{\text{top}} = 1$ but $C_{\text{eff}} = C_{\text{2body}} = 0$. The many-body calculation considers the complete quantum state and thus the correct transition amplitudes enter the Berry connection. Hence, we conclude from the agreement of the effective approach with the two-body approach that the effective approach is able to assess the Berry curvature and thus the Chern numbers of the many-body problem *without* conducting an extensive calculation in the complete Hilbert space. The deviating topological approach, while being justified for the ground state of fermionic models with filled bands, is not appropriate for determining the Berry curvature of excitations above the ground state.

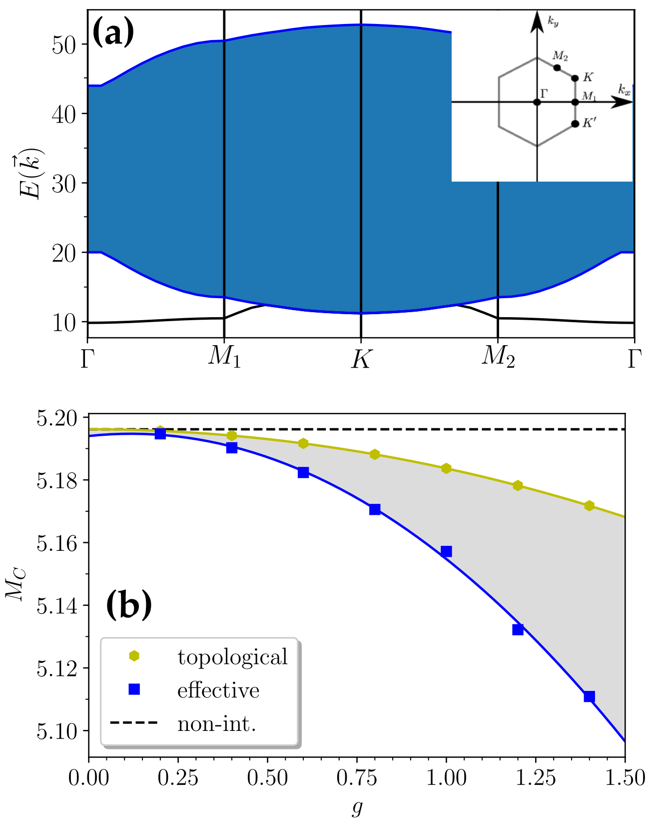

FIG. 2. (a) Two-boson continuum (colored) and renormalized single-boson bands for $E_0 = 16$, $M = 5.2$, and $g = 1.4$. (b) Critical values of M_C where the gap closes. Lines are quadratic fits.

The finding, that the effective Hamiltonian including the self-consistency yields exactly the same Berry phases and thus Chern numbers as considering the full Hilbert space, is analytically shown by the following argument. If the total Hilbert space $\mathcal{H}$ can be split into the direct sum of a single-particle part $\mathcal{H}(1)$ and the rest $\mathcal{H}_{\text{rest}}$ so that $\mathcal{H} = \mathcal{H}(1) \oplus \mathcal{H}_{\text{rest}}$, then a generic eigenvector v consists of $v = v_1 + v_{\text{rest}}$. In the Supplemental Material [56] we show that v_1 can be found by solving the self-consistency (3b). Transporting v parallelly around a contour γ yields v' and $\langle v|v'\rangle = \exp(i\varphi)$ implies $v' = \exp(i\varphi)v$ and the Berry phase φ. Thus, in $\mathcal{H}(1)$ the relation $v_1' = \exp(i\varphi)v_1$ holds so that the Berry phase determined in the subspace $\mathcal{H}(1)$ is identical to the one in the total Hilbert space.

In addition, we checked the bulk-boundary correspondence by inspecting the IPR. In case (i) we find clear numerical evidence that localized edge modes exist where the Chern number is different from zero; this is also confirmed by the LDOS, see Supplemental Material [56].

We find the same qualitative behavior if the upper band overlaps with the continuum, but not the lower band. Then the Chern number of the lower band is still unambiguously defined and the bulk-boundary correspondence holds.

Case II: Overlap with both bands. If both bands overlap with the continuum as shown in Fig. 2 for $E_0 = 16$ and $M = 5.2$, then it is not *a priori* clear if topological properties survive. The topological approach still works as before and yields the upper curve M_C in Fig. 2(b). But in the two other approaches we encounter major differences to the previous case. In the effective approach, the self-energy becomes non-Hermitian, but the effective Hamiltonian still defines two bands. Their eigenvalues are sufficiently separated in the complex plane so that the eigenvectors are defined unambiguously, except where the gap closes (5), yielding the lower curve in Fig. 2(b). We found numerical evidence that at gap closure, i.e., for $E_1(\vec{k}) = E_2(\vec{k})$, the Chern number changes and that this point is an exeptional point where both eigenvectors point in the same direction, see Supplemental Material [56]. Calculating the Chern numbers, we find that $C_{\text{top}} = C_{\text{eff}} = 1$ below the gray shaded area in Fig. 2(b), $C_{\text{top}} = 1$ and $C_{\text{eff}} = 0$ within the shaded area, and $C_{\text{top}} = C_{\text{eff}} = 0$ above.

The two-body approach in the full Hilbert space encounters the problem of a unique identification of the dressed single-boson states. We attempted to identify them by (a) maximizing the single-particle weight or by (b) maximizing the overlap of adjacent eigenvectors as function of wave vector in the BZ. But no reliable and numerical robust approach could be established. Hence, we cannot check independently whether the Chern number determined from the effective Hamiltonian has a physical meaning in the full Hilbert space. In addition, we investigated the existence of localized edge modes for nonzero effective Chern number. Both the IPR and the LDOS indicate that the potential edge modes delocalize since they are not protected by an energy gap for overlapping bands, see the Supplemental Material [56]. Hence, bands overlapping with continua appear to lose their particular topological properties, in line with the scenario on the single-particle level [36,37] in the absence of protecting energy gaps.

Conclusions. We have studied the topological properties of an interacting bosonic model on the honeycomb lattice allowing for the decay of a boson to two bosons and the inverse fusion. While the ground state (vacuum) is topologically trivial, the excited states are not. We investigated how Chern numbers C can be defined for these states and if edge states exist for nonvanishing C.

If the single-boson states are renormalized by the continuum without overlap in energy, then Chern numbers can be computed either in the many-body Hilbert space with the full Hamiltonian or in the single-boson space with the bilinear Hamiltonian plus the self-consistent self-energy (effective Hamiltonian). It is the first key finding that these two approaches agree while taking the self-energy at zero energy does not agree. This agreement of the effective self-consistent calculation with the correct Berry phases is corroborated by an analytic derivation. Furthermore, our results indicate that the bulk-boundary correspondence holds in this case.

If both single-boson bands lie energetically *within* the two-boson continuum, then one can extend the effective determination to the non-Hermitian case. The Chern number changes at gap closure which turns out to be an exceptional point. In spite of intensive search, we could not establish a robust definition of Berry phases in the full many-body Hilbert space. This sheds doubts on the significance of nontrivial Chern numbers in case of energetic overlaps. These doubts are enhanced by the absence of edge modes indicated by our numerical results of vanishing IPR and delocalized LDOS.

Our findings put the concept of nontrivial topology on a firm ground in the presence of interactions inducing continua. If the eigenstates are only renormalized by the hybridization with continua, then Chern numbers and the bulk-boundary correspondence apply as in the noninteracting case. If the single-particle states overlap with many-particle continua, then the concept of Chern numbers can be extended to non-Hermitian effective Hamiltonians. However, the Chern numbers are no longer protected by energy gaps and no localized edge modes seem to exist. This implies that an unambiguous definition of Berry phases in the full Hilbert space is no longer possible.

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