Topological Mott transition in a Weyl-Hubbard model with dynamical mean-field theory

Bernhard Isigler, 1 Tobias Grass, 2 Jun-Hui Zheng, 3 Mathieu Barbier, 1 and Walter Hofstetter 1

1 Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt am Main, Germany
2 ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain
3 Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

Weyl semimetals are three-dimensional, topologically protected, gapless phases which show exotic phenomena such as Fermi arc surface states or negative magnetoresistance. It is an open question whether interparticle interactions can turn the topological semimetal into a topologically nontrivial Mott insulating phase. We investigate an experimentally motivated model for Weyl physics of cold atoms in optical lattices, with the main focus on interaction effects and topological properties by means of dynamical mean-field theory (DMFT). We characterize topological phases by numerically evaluating the Chern number via the Ishikawa-Matsuyama formula for interacting phases. Within our studies, we find that the Chern numbers become trivial when interactions lead to insulating behavior. For a deeper understanding of the Weyl-semimetal-to-Mott-insulator topological phase transition, we evaluate the topological properties of quasiparticle bands as well as so-called blind bands. Our study is complementary to recent studies of Weyl semimetals with DMFT.

I. INTRODUCTION

Topological states of matter realized with cold atoms in optical lattices are a vibrant field at the forefront of modern quantum research. The great control and tunability of cold atoms in optical lattices make them an ideal analog quantum simulator of tight-binding Hamiltonians. Among pioneering experiments in the context of topological states are the realizations of two prominent theoretical two-dimensional (2d) models: the Hofstadter model 3 and the Haldane model. 4 The former is realized by imprinting a complex quantum phase onto the particles upon hopping in the lattice through laser-assisted tunneling. The latter is engineered through elliptic lattice shaking which also imprints a complex phase according to Floquet’s theorem. Both approaches are well described by effective static Floquet Hamiltonians with gauge fields as a result of high-frequency driving.

The current focus of research in this field clearly lies in 2d systems. One reason is the fact that 2d systems host paradigmatic phases such as the quantum Hall effect. The possible existence of topological phases is connected to the dimensionality and symmetries of the system of interest. In contrast to 2d, in three-dimensional (3d) systems, even gapless states can be topologically protected. Examples are the Weyl semimetal (WSM) and nodal-line semimetals. Moreover, the search for an exotic topological Mott insulator suggested its existence in 3d optical lattices.

WSMs host gapless Weyl points (WPs) in the 3d Brillouin zone (BZ) which are topologically protected, i.e., they cannot gap out through smooth deformations of the Hamiltonian. One generally differentiates between WSMs with broken time-reversal symmetry or WSMs with broken inversion symmetry. If both are broken, the WPs are not located at the Fermi level. WSMs have first been observed in 2015 in a TaAs crystal along with the exotic Fermi arc surface states by means of photoemission spectroscopy as well as in a gyroid photonic crystal both with broken inversion symmetry. Another intriguing feature of WSMs is the chiral anomaly and the resulting negative magnetoresistance which was also measured in TaAs crystals. Recently, a nodal-line semimetal has been engineered as the first instance of a 3d topological state in a cold atom setup, but the realization of an atomic WSM is still lacking.

In the interacting case, the Weyl-Mott insulator has been proposed as an extension to the noninteracting WSM. The model has a momentum-locked interaction and is analytically solvable. This is possible through the assumption of this particular form of the interaction. Moreover, the system has a Mott gap as well as a nontrivial topological invariant in terms of the single particle Green’s function. Ref. pointed out that this invariant does not imply the presence of a single-particle Fermi arc because of the absence of the WPs in the single-particle spectrum. Instead, the system has gapless particle-hole pair excitations, suggesting the existence of the Weyl points in the bosonic excitation spectrum. The nonzero topological invariant indeed implies the presence of a bosonic surface state. While a single-particle Fermi arc is observable through photoemission spectroscopy, the bosonic surface is not accessible with photoemission spectroscopy.

In Ref. the interactions which give rise to the Weyl-Mott insulator are local in momentum space, whereas in realistic systems, the interactions are rather local in real space. In the present paper, we investigate the effect of realistic on-site interactions on a WSM. To analyze the topological properties of such a system, we compute the topological invariants in terms of the single-particle Green’s function. In most cases, this quantity is well suited to examine the topologically non-trivial behavior. This evaluation is particularly useful when the many-body wavefunction is numerically not accessible. We use
dynamical mean-field theory (DMFT) in order to solve the present many-body problem approximately. In the context of topological systems, DMFT has been used in numerous studies in 2D as well as 3D systems. DMFT has been applied recently to WSMs: In Ref. the nonlocal annihilation of WPs within the BZ has been observed which is impossible in the noninteracting case. Ref. on the other hand, investigated the influence of interactions in view of the negative magnetoresistance. Our focus lies on the topological properties of the many-body phases which we obtain. We find that the WSM is robust up to a critical interaction strength. In particular, we observe that the transition from a topologically nontrivial WSM to a trivial Mott insulator occurs through the emergence of pairs of quasiparticle bands and so-called blind bands. Here, the former are topologically nontrivial and cancel out the nontrivial properties of the original WSM while the latter are topologically trivial. This ultimately results in an overall topologically trivial Mott insulator.

The article is structured as follows: In Sec. we introduce the model for a WSM and investigate its noninteracting properties. In Sec. we analyze the WSM-to-Mott-insulator transition of the interacting model. In Sec. we compute topological properties as a function of the interaction strength. In Sec. we discuss the effective quasiparticle spectrum and elaborate on the interaction-induced WSM-to-Mott-insulator topological phase transition. Finally, we conclude in Sec. VI.

II. MODEL

We study the tight-binding model proposed by Dubček et al. which is motivated by the experimental implementation of the Hofstadter model in Ref. extended to three spatial dimensions. The corresponding real-space Hamiltonian reads

\[
\hat{H}_{\text{Dubček}} = -\sum_j \left[ (-1)^{x+y} K_x \hat{c}_j^\dagger \hat{c}_{j+x} + J_y \hat{c}_j^\dagger \hat{c}_{j+y} + h.c. \right] + (-1)^{x+y} K_z \hat{c}_j^\dagger \hat{c}_{j+z} + h.c. \right]
\]

(1)

where \( j = (x, y, z) \) is a 3d lattice vector on a cubic lattice, \( \hat{c}_j \) \((\hat{c}_j^\dagger)\) annihilates (creates) a fermion at lattice site \( j \), and \( \hat{\nu} \) denotes the unit vector in \( \nu \) direction. In the following, we focus on the isotropic case and set the hopping energies to the unit of energy \( K_x = J_y = K_z = 1 \). The momentum-space Hamiltonian reads

\[
H_{\text{Dubček}}(k) = -2 \left[ \cos(k_y) \sigma_x \sigma^x + \sin(k_z) \sigma^y \sigma^y - \cos(k_x) \sigma^z \right]
\]

(2)

where we have set the lattice constant to unity. Here, the Pauli matrices \( \sigma^\nu \) refer to the pseudo-spin space of the two sites of the unit cell which breaks inversion symmetry. We read off four degeneracies of the Hamiltonian in Eq. at the points \( (k_x, k_y, k_z) = (0, \pm \pi/2, \pm \pi/2) \) in the first BZ. To confirm whether these degeneracies are indeed WPs, we compute the Chern number on a closed surface around a single degeneracy using Fuku’s method. In fact, any smooth closed surface can be used, see appendix A. Indeed, the four closed points \( (0, \pm \pi/2, \pm \pi/2) \) exhibit nonzero Chern numbers (+1 or -1), also dubbed topological charge. The sum over the four topological charges is zero.

III. MOTT TRANSITION

Let us now focus on the properties of the Mott transition of the model in Eq. (1). We consider fermions with a Hubbard interaction term \( U \sum_j \hat{n}_{j \uparrow} \hat{n}_{j \downarrow} \) where \( U \) is the interaction strength and \( \hat{n}_{j \sigma} = \hat{c}_j^\dagger \hat{c}_{j \sigma} \) is the particle number operator of a spin-\( \sigma \) fermion on lattice site \( j \).

Spin states are introduced in the following way in the four-band interacting Hamiltonian:

\[
\hat{H}_{\text{int}} = \begin{pmatrix} \hat{H}_{\text{Dubček}} & 0 \\ 0 & \hat{H}_{\text{Dubček}} \end{pmatrix} + U \sum_j \hat{n}_{j \uparrow} \hat{n}_{j \downarrow}
\]

(3)

The spin degeneracy results in a factor of 2 for the topological charges of the WPs.

One of the most successful methods for investigating Hubbard-like Hamiltonians and describing their Mott transitions is DMFT. It maps the full Hubbard model onto a set of coupled self-consistent quantum impurity models which can be solved through different approaches like quantum Monte Carlo or exact diagonalization (ED). This mapping neglects nonlocal fluctuations but keeps track of all local quantum fluctuations. This manifests in a momentum-independent selfenergy \( \Sigma_{\sigma \sigma'}(\omega, k) = \Sigma_{\sigma \sigma'}(\omega) \) with \( \sigma \) and \( \sigma' \) denoting spin states. As in static mean-field theories, DMFT is solved self-consistently and thus depends on an initial guess.

Here, we perform real-space DMFT calculations on a 6 × 6 lattice for the model in Eq. (2) with an ED solver with four bath sites. We are interested in the paramagnetic case. The paramagnetic solution is sufficient to describe the Mott transition. Besides, the temperature regimes we consider are above the superexchange temperature for antiferromagnetic ordering. The paramagnetic solution is found if diagonal elements of the selfenergy in spin space are identical and off-diagonal elements vanish:

\[
\Sigma_{\uparrow \downarrow}(\omega) = \Sigma_{\downarrow \uparrow}(\omega) = \Sigma(\omega)
\]

(4)

\[
\Sigma_{\uparrow \uparrow}(\omega) = \Sigma_{\downarrow \downarrow}(\omega) = 0
\]

(5)

The Hamiltonian in Eq. (3) is symmetric under the translations \( j \rightarrow j + \hat{z} \) and \( j \rightarrow j + \hat{x} + \hat{y} \). It is then sufficient to compute only two separate local selfenergies, i.e., solving two separate impurity problems, and copy them accordingly in the lattice Green’s function.

As indicators for the Mott transition, we compute two quantities: (i) the double occupancy

\[
n_d = \frac{1}{N_s} \sum_j \langle \hat{n}_{j \uparrow} \hat{n}_{j \downarrow} \rangle
\]

(6)
The critical interaction strength for this phase transition with \( \Sigma(\omega) \) and the selfenergy for the DMFT calculations is labeled by up and down. The hysteresis between these is highlighted by a shaded area. Energies are measured in units of the hopping energy.

where \( N_s \) is the number of lattice sites and \( \langle \ldots \rangle \) denotes the ensemble average; (ii) the quasiparticle weight \( Q \) defined as

\[
Q = \left[ 1 - \frac{\partial \Sigma(\omega)}{\partial \omega} \right]^{-1} = \left[ 1 - \frac{\Sigma(i\omega_n)}{i\omega_n} \right]^{-1} \tag{7}
\]

where we have introduced the real-frequency selfenergy \( \Sigma(\omega) \) and the selfenergy in terms of Matsubara frequencies \( \Sigma(i\omega_n) \). We present the results for \( n_d \) and \( Q \) in Fig. 1 as functions of the interaction strength \( U \) for different temperatures. The self-consistent solutions are found successively for different \( U \). The initial guess for the self-consistent DMFT iteration is inherited from the previous converged solution for the previous value of \( U \). Starting with \( U = 0 \), i.e., going upwards, the first guess for the initial selfenergy is zero. For the downwards calculations, the deep Mott solution at \( U = 20 \) was used which was previously found by the upwards calculation. As the difference between those curves, we observe the typical hysteresis of the paramagnetic solutions shown as shaded areas. The hysteresis reflects the coexistence of two solutions, i.e., the correlated WSM and the Mott insulator. The critical interaction strength for this phase transition is located within this coexistence regime. As we observe in Fig. 1, this regime is temperature dependent, and thus also the critical interaction strength. For comparison, the critical interaction strength for the metal-to-Mott-insulator transition in the 3d Hubbard model at \( T \approx 0.33 \) is \( U = 15.4 \).

To determine transport properties of the obtained many-body phases, we are interested in the density of states

\[
A(\omega) = -\frac{1}{\pi} \text{Im} \int d\mathbf{k} \text{Tr} G(\omega, \mathbf{k}) \quad \tag{8}
\]

where we have defined the retarded, real-frequency single-particle Green’s function

\[
G(\omega, \mathbf{k}) = \frac{1}{\omega + \Sigma(\omega) + \mu I - H(\mathbf{k})}, \quad \tag{9}
\]

which does only apply for the paramagnetic solutions. Here, \( I \) denotes the \( 2 \times 2 \) identity matrix in the sublattice representation, and \( \mu \) is the chemical potential which is set to \( U/2 \) throughout the article, constraining the system to be half-filled. In Fig. 2, we show the density of states for different \( U \) at \( T = 0.1 \). For \( U = 1 \), the density of states is almost identical to the one of the noninteracting case \( U = 0 \). This is expected since the selfenergy is small in this regime. We also observe the peaks from the two bands of the Hamiltonian and an approximately quadratic behavior around \( \omega = 0 \) which is a property of a semimetal. For \( U = 10 \), we observe two Hubbard bands at approximately \( \omega = \pm 8 \). The bands close to \( \omega = 0 \) are shrunk compared to the \( U = 1 \) case but the system is still semimetallic. For \( U = 20 \), we find an overall gap of size \( \sim 16 \) which corresponds to the Mott gap. The structure of each of the Hubbard bands resembles the structure of the original density of states at \( U = 0 \). Such splitting of the noninteracting bands, each with the density of states similar to the noninteracting one, has been observed before in a bosonic system.

In Eq. (9), the selfenergy in terms of real frequencies \( \omega \) enters. Most impurity solvers, however, provide the output as a function of Matsubara frequencies \( i\omega_n \). Here, we use the maximum entropy method in order to map \( \Sigma(i\omega_n) \) to \( \Sigma(\omega) \). This method was originally developed to analytically continue noisy quantum Monte Carlo data. It has the advantage to yield smooth outcomes through Bayesian statistics. Here, we use this method to analytically continue ED results. Conventionally, the density of states from ED calculations is rugged due to the finite number of bath sites. Here, the maximum entropy method can compensate that. Of course, the result is then approximate. The results in Fig. 2 show that our approach of combining the maximum entropy method with ED results yields a reasonable outcome.

In summary, the double occupancy, the quasiparticle weight, and the density of states provide clear evidence that the many-body phase for strong \( U > 15 \) is a Mott insulator. Let us now turn to the topological properties...
of the interacting system.

IV. ISHIKAWA-MATSUYAMA FORMULA

The Ishikawa-Matsuyama formula manifests the generalization of a Chern number to interacting systems as it corresponds to the Hall conductivity up to a constant factor and is formulated in terms of Green’s function:

\[ C_{\text{IM}} = \frac{e^{\nu \rho n}}{24\pi^2} \int dk \text{Tr} \left\{ \left[ G \partial_{\nu} G^{-1} \right] \left[ G \partial_{\rho} G^{-1} \right] \left[ G \partial_{\eta} G^{-1} \right] \right\} \]

(10)

where \( k = (k_0, k_1, k_2) \) with \( k_0 = i\omega_n \) and \( \nu, \rho, \eta \) run over the elements of \( k \). We also have used the abbreviation \( G = G(k) = G(i\omega_n, k_1, k_2) \). The formula is rather complicated compared to the noninteracting TKNN invariant. It has been shown, however, that in some regimes the information about the full frequency range is not necessary and only the \( \omega = 0 \) mode is crucial. This is called the effective topological Hamiltonian approach which makes it possible to compute topological invariants from an effective, noninteracting Hamiltonian \( H_{\text{top}} = -G^{-1}(\omega = 0, k) \). This, however, is valid only if the Green’s function has no zeros which is of course not the case in a Mott insulator.

For the sake of brevity, we drop all the arguments. So, we find

\[ \partial_{k_\nu} G^{-1} = (1 - \partial_{k_\nu} \Sigma) \mathbb{I} = (1 + i\partial_{\omega_n} \Sigma) \mathbb{I} \]

(12)

\[ \partial_{k_\nu} G^{-1} = \partial_{k_\nu} H = j_\nu \]

(13)

where \( j_\nu = j_\nu(k_1, k_2) \) is the current in \( \nu = 1, 2 \) direction with the 2d momenta \( k_1 \) and \( k_2 \). Consequently, Eq. (10) simplifies to

\[ C_{\text{IM}} = \frac{i}{8\pi^2} \int dk_1 dk_2 d\omega_n \times \text{Tr} \left\{ G_{j_1} G_{j_2} G (1 + i\partial_{\omega_n} \Sigma) \right\} \]

(14)

Following the above discussion of the noninteracting case, see also appendix A, we will put the 2d momentum \((k_1, k_2)\) onto a surface enclosing the WPs in the 3d BZ of the interacting system to compute topological charges of the WPs in the interacting case.

The momentum-dependent part of the formula in Eq. (14) can be calculated analytically depending on the surface enclosing the WP over which we want to integrate. For the two components of the currents, this implies

\[ j_r = \sum_\nu j_\nu \frac{\partial k_\nu}{\partial k_r}, \quad r = 1, 2 \quad \text{and} \quad \nu = x, y, z. \]

(15)

V. QUASIPARTICLE SPECTRUM AND BLIND BANDS

It is anticipated that the topological invariant on the enclosing surface vanishes when the WPs gap out since the system then lacks the singularity which has to be enclosed, compare Figs. 2 and 3. The resulting many-body state is globally gapped. Due to the lack of WPs...
there are neither sources nor sinks of Berry curvature. The many-body state is thus topologically trivial. For finite magnetization, topologically trivial states have been found.

We want to understand in more detail how this topological phase transition to a topologically trivial Mott insulator occurs. To this end, we again focus on the paramagnetic case. Our conventional understanding of topological phase transitions is the closing of a quasiparticle band gap. Quasiparticle bands exhibit Chern numbers and correspond to the poles of the single-particle Green’s function. It has been discussed, however, on the level of single-particle Green’s functions, that not only poles of the Green’s function can exhibit nontrivial Chern numbers but also zeros of the Green’s function. The zeros of the Green’s function are dubbed blind bands. Ref. [60] proposed the interaction-induced topological phase transition through a gap closing of blind bands. Herein, not only the quasiparticle bands, but also the blind bands exhibit nontrivial Chern numbers. The gap closing of blind bands then can induce a topological phase transition. In our case, we do not find nontrivial blind bands but rather a topological phase transition stemming from the quasiparticle bands only.

The topological properties of the interacting system are described by a formula for a generalized Chern number $\tilde{C}$ which relates the Chern numbers of quasiparticle bands and the Chern numbers of blind bands and was derived from the Ishikawa-Matsuyama formula[23]

$$\tilde{C} = \sum_{n=1}^{N} \int dk_1 dk_2 \text{Im}(-\partial_{k_1} \text{Im}(\omega_n^p(k), k) \partial_{k_2} \text{Im}(\omega_n^p(k), k))$$

$$- \sum_{m=1}^{M} \int dk_1 dk_2 \text{Im}(-\partial_{k_1} \text{Im}(\omega_m^z(k), k) \partial_{k_2} \text{Im}(\omega_m^z(k), k))$$

(17)

Herein, we have defined the eigenstates $|\psi_j(\omega, k)\rangle$ of the Green’s function according to

$$G(\omega, k)|\psi_j(\omega, k)\rangle = g_j(\omega, k)|\psi_j(\omega, k)\rangle.$$  

(18)

Since the Green’s function is not hermitian away from $\omega = 0$, the eigenvalues $g_j(\omega, k)$ are not real in general and there is no generic ordering. Since we are only interested in zeros and poles of $g_j(\omega, k)$, we order the eigenvalues by their absolute values. In Eq. (17), we have also defined the quasiparticle bands $\omega_n^p(k)$ and the blind bands $\omega_m^z(k)$ as the poles and zeros of the Green’s function, respectively:

$$g_j(\omega = \omega_n^p(k), k) \to \infty \quad \text{and} \quad g_j(\omega = \omega_m^z(k), k) = 0.$$  

(19)

We have dropped the band index $j$ for the states in Eq. (17) since $j$ is fully determined by $\omega_n^p(k)$ and $\omega_m^z(k)$, respectively. Furthermore, we focus on the weakly interacting case and the deep Mott-insulating case. In the intermediate regime, the poles and zeros are not sufficiently pronounced. Note that the physics in the deep Mott regime will certainly differ from this treatment as, e.g., particle-hole excitations are neglected. We emphasize that our discussion focuses on the framework of single-particle Green’s functions.

We show the absolute value of the eigenvalues of the Green’s function in log scale exemplarily for a specific $k$ on the WP-enclosing sphere.

![FIG. 4. Absolute value of the eigenvalues of the Green’s function in log scale exemplarily for a specific $k$ on the WP-enclosing sphere.](image)
We compute two new quantities derived from the density of states as a function of the polar angle. Values as a function of the polar angle are plotted implicitly. A continuous flattening of the quasiparticle bands. Instead, the topological phase transition occurs through a closing of the quasiparticle gap by a continuous flattening of the semimetallic quasiparticle bands. Both indicates a closing of a quasiparticle gap as well as a flattening of the semimetallic quasiparticle bands. This ultimately, enables the nonlocal annihilation of the Weyl points. The flat blind bands do not contribute to the topological properties of the system.

VI. CONCLUSION

We have investigated an experimentally relevant model in the field of cold atoms in optical lattices by means of DMFT. We have calculated the double occupancy, the quasiparticle weight, as well as the density of states to determine a paramagnetic Mott insulating phase for strong Hubbard interactions. Through numerical evaluation of the Ishikawa-Matsuyama formula, which is more general than the effective topological Hamiltonian approach, we have determined the topological WSM-to-Mott-insulator transition. We investigated this topological phase transition in further detail by extracting quasiparticle bands and blind bands which both can carry Chern numbers. It turns out that the topological phase transition occurs through a closing of the quasiparticle band gap by a continuous flattening of the semimetallic quasiparticle bands. This ultimately, enables the nonlocal annihilation of the Weyl points. The flat blind bands do not contribute to the topological properties of the system.

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Appendix A: Chern number in curvilinear coordinates

Here, we show that the analytical form of the Chern number stays invariant in an arbitrary 3d curvilinear coordinate system. We transform the expression for the Chern number which is typically defined in the cartesian BZ \((k_x, k_y, k_z)\) to the curvilinear coordinate system \((k_1, k_2, k_3)\). The flux element reads

$$BdS = dS \cdot \partial_k \times A$$  \hspace{1cm} (A1)$$

where \(A = i\langle \psi|\partial_k|\psi\rangle\) is the Berry connection with \(\partial_k\) being the nabla operator and \(|\psi\rangle\equiv|\psi(k)\rangle\) being the \(k\)-dependent Bloch state. We express the Berry connection in curvilinear coordinates

$$A = i\langle \psi|\partial_k|\psi\rangle \frac{\hat{e}_r}{h_r}$$  \hspace{1cm} (A2)$$

where \(h_r = |h_r|\) is the Lamé factor where \(h_r = (\partial_{k_r} h_r)\hat{e}_r\) with \(\nu = x, y, z\) running over the cartesian coordinates and \(r = 1, 2, 3\) running over the curvilinear coordinates. Here, \(\hat{e}_r\) is the unit vector in \(k_r\) direction and \(\hat{e}_s\) is the unit vector in \(k_s\) direction. The Lamé factor is related to the metric tensor as \(g_{rs} = h_r \cdot h_s\).

Now, we express the curl in curvilinear coordinates

$$\partial_k \times A = \frac{\epsilon^{rst}}{h_s h_t} (\partial_{k_r} h_s A_s) \hat{e}_t$$  \hspace{1cm} (A3)$$

for the sphere

$$\begin{bmatrix}
    k_x(	heta_S, \phi_S) \\
    k_y(	heta_S, \phi_S) \\
    k_z(	heta_S, \phi_S)
\end{bmatrix} = k_{WP} + R_S \begin{bmatrix}
    \sin(\theta_S) \cos(\phi_S) \\
    \sin(\theta_S) \sin(\phi_S) \\
    \cos(\theta_S)
\end{bmatrix}$$  \hspace{1cm} (A10)$$

and for the torus

$$\begin{bmatrix}
    k_x(\theta_T, \phi_T) \\
    k_y(\theta_T, \phi_T) \\
    k_z(\theta_T, \phi_T)
\end{bmatrix} = k_{WP} + R_T \begin{bmatrix}
    \cos(\phi_T) \\
    \sin(\phi_T) \\
    0
\end{bmatrix} + r_T \begin{bmatrix}
    \cos(\theta_T) \cos(\phi_T) \\
    \cos(\theta_T) \sin(\phi_T) \\
    \sin(\theta_T)
\end{bmatrix}$$  \hspace{1cm} (A11)$$

where \(k_{WP}\) denotes the position of the WP in the BZ. The Chern number, or topological charge, then follows by substituting \((\theta_S, \phi_S)\) and \((\theta_T, \phi_T)\), respectively, for \((k_1, k_2)\) in Eq. \(A9\). Note that for the torus, \(k_{WP}\) has to be shifted, e.g., by \(R_T \hat{e}_r\), in order to properly enclose the WP. The results for the Berry curvature as a function of \((\theta_S, \phi_S)\) and \((\theta_T, \phi_T)\), respectively, are shown in Fig. 7 for the model in Eq. \(2\). Integrating these Berry curvatures yields 1 and -1, respectively, according to the two different WPs enclosed. For the sphere, we have used \(k_{WP} = (0, \pi/2, -\pi/2)\) and \(R_S = \pi/2\) and for the torus we have used \(k_{WP} = (-R_T, \pi/2, \pi/2)\), \(R_T = \pi/6\), and \(r_T = \pi/6\).
Appendix B: Real-valuedness of the Ishikawa-Matsuyama formula

The invariant in Eq. (14) is purely real. To show this, we reintroduce the frequency argument and define

\[ \Lambda_1(i\omega_n) = G(i\omega_n) j_1 G(i\omega_n) j_2 G(i\omega_n) (1 + i\partial_n \Sigma(i\omega_n)) \]

(B1)

\[ \Lambda_2(i\omega_n) = (1 + i\partial_n \Sigma(i\omega_n)) G(i\omega_n) j_2 G(i\omega_n) j_1 G(i\omega_n) \]

(B2)

which yields

\[ C_{\text{IM}} = \frac{i}{8\pi^2} \int dk d\omega_n \text{Tr} [\Lambda_1(i\omega_n) - \Lambda_2(i\omega_n)] \]

(B3)

Let us consider the hermitian conjugate of \( \Lambda_1 \):

\[ [G(i\omega_n) j_1 G(i\omega_n) j_2 G(i\omega_n) (1 + i\partial_n \Sigma(i\omega_n))]^\dagger \]

(B4)

\[ = (1 + i\partial_n \Sigma(i\omega_n))^\dagger G(i\omega_n) j_2^\dagger G(i\omega_n) j_1^\dagger G(i\omega_n) \]

(B5)

\[ = (1 - i\partial_n \Sigma(i\omega_n))^\dagger) G(-i\omega_n) j_2 G(-i\omega_n) j_1 G(-i\omega_n) \]

(B6)

\[ = (1 + i\partial_{-\omega_n} \Sigma(-i\omega_n)) G(-i\omega_n) j_2 G(-i\omega_n) j_1 G(-i\omega_n) \]

(B7)

\[ = \Lambda_2(-i\omega_n) \]

(B8)

where we have used the fact that the currents \( j_i \) are hermitian matrices as well as the symmetries of the Green’s function \( G(i\omega_n) = G(-i\omega_n) \) and the selfenergy \( \Sigma^*(i\omega_n) = \Sigma(-i\omega_n) \). We thus find that Eq. (B3) can be rewritten as

\[ C_{\text{IM}} = \frac{i}{8\pi^2} \int dk d\omega_n \text{Tr} \left[ \Lambda_1(i\omega_n) - \Lambda_1^*(i\omega_n) \right] \]

(B9)

which is purely real. From the first line to the second line, we have used that we integrate over the full frequency range. In the third line we have expressed the trace of \( \Lambda_1(i\omega_n) \) in terms of its eigenvalues \( \lambda_l(i\omega_n) \).