Chern number and Berry curvature for Gaussian mixed states of fermions

Lukas Wawer and Michael Fleischhauer
Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

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We generalize the concept of topological invariants for mixed states based on the ensemble geometric phase (EGP) to two-dimensional band structures. In contrast to the geometric Uhlmann phase for density matrices, the EGP leads to a proper Chern number for Gaussian, finite-temperature, or nonequilibrium steady states. The Chern number can be expressed as an integral of the ground-state Berry curvature of a fictitious lattice Hamiltonian, constructed from single-particle correlations. For the Chern number to be nonzero the fictitious Hamiltonian has to break time-reversal symmetry.

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I. INTRODUCTION

Transitions between different phases of quantum matter are characterized either by a spontaneous breaking of symmetries or by changes in the topology of the many-body ground state [1–3]. Topologically different phases can be distinguished by invariants, which identify global properties of the system. The existence of these integer quantum numbers is also the origin of the robustness of characteristic features such as edge states and currents or quantized bulk transport [4–8]. Typical topological invariants are based on geometric phases such as the Berry or Zak phase [1] which characterize the parallel transport of the many-body ground state upon cyclic changes in system parameters. They are thus applicable only to pure states. Several attempts have been made over the last years to extend the concept of topological invariants to mixed states of noninteracting fermions [9–20] with the aim of classifying finite-temperature or nonequilibrium steady states. Although some aspects of topology in open quantum systems can be captured by non-Hermitian Hamiltonians [21–23], a proper classification must account for both dissipation and fluctuations and requires the discussion of density matrices.

A possible generalization of the Berry phase to density matrices was given by Uhlmann [24]. Based on Uhlmann's construction a mixed-state topological invariant for one-dimensional (1D) systems was defined in Ref. [12] as the winding number of the Uhlmann phase upon cyclic parameter changes. For 1D lattice systems in a gapped *ground* state, the Uhlmann phase is identical to the Zak phase. In this limit its winding can thus be expressed as an integral of a Berry curvature over a 2D torus (lattice momentum and time), which is the well-known first Chern number. For mixed states the existence of a proper Berry connection is in general, however, not guaranteed. As shown in Ref. [16] the approach based on the Uhlmann phase fails when applied to two dimensions [13,14]. The windings of the Uhlmann phases in the x and y directions, $\int dk_x \partial_{k_x} \phi_y^U(k_x)$ and $\int dk_y \partial_{k_y} \phi_x^U(k_y)$, are for some parameters not the same, demonstrating that no proper Berry connection exists.

Recently, we have shown that a generalization of Resta's many-body polarization [25] to mixed states, termed the ensemble geometric phase (EGP) [17,18], is an alternative way to define a topological invariant for Gaussian states of fermions in one dimension. In the thermodynamic limit the EGP approaches the Zak phase of the lowest band of a single-particle Bloch Hamiltonian, termed a fictitious Hamiltonian, which is defined by single-particle correlations and thus contains all properties of the Gaussian mixed state. The winding number of the EGP is a topological invariant characterizing this fictitious Hamiltonian. The EGP can be detected, and a nontrivial topology has direct physical consequences such as quantized particle transport in an auxiliary system weakly coupled to the fermion chain [26]. It can also be extended to 1D models with interactions including systems with fractional topological charges [27].

As is the case for the Uhlmann phase, the EGP depends on the choice of the momentum direction, when considering two-dimensional lattice models. However, as will be shown here, and in contrast to the Uhlmann case, the EGP in any spatial direction can be expressed as a closed-loop integral over the corresponding component of a *single* Berry connection. The latter describes the ground-state wave function of the fictitious Bloch Hamiltonian. Thus based on the EGP one can define a unique Chern number for mixed states in two dimensions. To illustrate this, we discuss the asymmetric Qi-Wu-Zhang model, which is a two-dimensional, topologically nontrivial lattice model with two bands. Due to the asymmetry of the band structure the winding of the Uhlmann phase is different in the x and y directions in a certain range of temperatures [16]. The EGP winding, on the other hand, is always the same in all directions.

II. BERRY CURVATURE AND ZAK PHASE

To set the stage, we start by shortly summarizing the topological classification of fermions in terms of the Berry curvature of Bloch states. To this end, we consider insulating many-body states of noninteracting fermions on a two-dimensional lattice described by a number-conserving Hamiltonian. We set the lattice constant $a = 1$, consider a total number of N^2 unit cells with periodic boundary conditions in the x and y directions, and use $\hbar = 1$. The operators $\hat{c}_{\boldsymbol{j},\lambda}, \hat{c}^\dagger_{\boldsymbol{j},\lambda}$ describe the annihilation and creation of a fermion in the $\boldsymbol{j}$th unit cell. $\boldsymbol{j} = (j_x, j_y)$ denotes the x and y coordinates of the unit cell, respectively, and the index $\lambda \in \{1, \dots, p\}$ labels a possible internal degree of freedom within a unit cell. Assuming translational invariance for simplicity, the Hamiltonian can be written in second quantization as

$$H = \sum_{\boldsymbol{k}} \sum_{\mu,\nu=1}^{p} \tilde{c}^\dagger_\lambda(\boldsymbol{k})\, \mathsf{h}_{\mu\nu}(\boldsymbol{k})\, \tilde{c}_\nu(\boldsymbol{k}). \tag{1}$$

Here, $\boldsymbol{k} = (k_x, k_y)$ is the lattice momentum, and h is the $p \times p$ single-particle Hamiltonian matrix in momentum space. We assume that h has multiple bands, separated by finite gaps, and we consider an insulator, i.e., assume that the chemical potential μ lies within a band gap.

If h breaks time-reversal symmetry, the topological properties of a gapped many-body state can be characterized by the Berry curvature $\mathcal{F}^{(n)}(\boldsymbol{k})$ of all occupied Bloch bands n:

$$\begin{aligned}\mathcal{F}^{(n)}(\boldsymbol{k}) &= (\nabla_k \times \boldsymbol{A}^{(n)}(\boldsymbol{k}))_z \\ &= i\big(\big\langle \partial_{k_x} u_n(\boldsymbol{k}) \big| \partial_{k_y} u_n(\boldsymbol{k})\big\rangle - \big\langle \partial_{k_y} u_n(\boldsymbol{k}) \big| \partial_{k_x} u_n(\boldsymbol{k})\big\rangle\big).\end{aligned} \tag{2}$$

Here, $|u_n(\boldsymbol{k})\rangle$ is the Bloch function of the nth band, and $\boldsymbol{A}^{(n)}(\boldsymbol{k})$ is the Berry connection $A^{(n)}_j(\boldsymbol{k}) = i\langle u_n(\boldsymbol{k})|\partial_{k_j} u_n(\boldsymbol{k})\rangle$. While the Berry curvature is not gauge invariant, its integral over the two-dimensional torus of the Brillouin zone is. It furthermore defines an integer-valued topological invariant of the band, the first Chern number

$$C = \frac{1}{2\pi} \oiint_{\mathrm{BZ}} d\boldsymbol{k}\, \mathcal{F}^{(n)}(\boldsymbol{k}). \tag{3}$$

The Chern number can also be related to the geometric phase picked up by a Bloch state $|u_n(\boldsymbol{k})\rangle$ upon parallel transport in momentum space through the Brillouin zone in either the k_x or k_y direction. It can be written in terms of the winding of the Zak phases, defined as

$$\phi^{\mathrm{Zak}}_x(k_y) = i \oint_{\mathrm{BZ}} dk_x \big\langle u(\boldsymbol{k}) \big| \partial_{k_x} u(\boldsymbol{k})\big\rangle = \oint_{\mathrm{BZ}} dk_x\, A_x(\boldsymbol{k}) \tag{4}$$

or $\phi^{\mathrm{Zak}}_y(k_x)$, respectively. Note that we have dropped the band index for simplicity. Most importantly, the two Zak phases in the x and y directions can be expressed as integrals of the components of a single vector, the Berry connection $\boldsymbol{A} = i\langle u(\boldsymbol{k})|\nabla_{\boldsymbol{k}} u(\boldsymbol{k})\rangle$. As a consequence the windings of the two phases

$$\begin{aligned}C_x &= \frac{1}{2\pi} \oint_{\mathrm{BZ}} dk_y \frac{\partial}{\partial k_y} \phi^{\mathrm{Zak}}_x(k_y), \\ C_y &= -\frac{1}{2\pi} \oint_{\mathrm{BZ}} dk_x \frac{\partial}{\partial k_x} \phi^{\mathrm{Zak}}_y(k_x)\end{aligned}$$

must be identical and equal to the Chern number

$$C_x = C_y = C. \tag{5}$$

III. GEOMETRIC PHASE FOR DENSITY MATRICES: UHLMANN CONSTRUCTION

Topological invariants for pure states, such as the Chern number, characterize how a gapped many-body state $|\psi\rangle$ changes upon parallel transport along a closed loop in parameter space. The parallel-transport requirement leads directly to the definition of the Berry phase, or for lattice systems to the Zak phase, Eq. (4). The corresponding Berry connection transforms as a U(1) gauge field according to $|u(\boldsymbol{k})\rangle \to e^{i\chi(\boldsymbol{k})}|u(\boldsymbol{k})\rangle$: $\boldsymbol{A} \to \boldsymbol{A} - \nabla_{\boldsymbol{k}}\chi(\boldsymbol{k})$.

A generalization of geometric phases to density matrices ρ was introduced by Uhlmann [24], who pointed out that the decomposition $\rho = w \cdot w^\dagger$ of an $n \times n$ density matrix into matrices w contains a gauge freedom $w \to w\,\mathsf{U}$, where U is a U(n) unitary matrix. Since ρ is positive semidefinite, w can always be represented as

$$w = \sqrt{\rho}\,\mathsf{U}. \tag{6}$$

Let $\rho = \rho(\lambda)$ be a uniquely defined mixed state, and let $\lambda \in \{0, \Lambda\}$ parametrize a closed loop in parameter space such that $\rho(0) = \rho(\Lambda)$. Requiring parallel transport of the density matrix in the generalization of Berry's construction, one can then define a U(n) Uhlmann holonomy

$$\mathcal{H}_{\mathrm{U}} = \mathsf{U}(\Lambda)\mathsf{U}^\dagger(0) = \mathcal{P}e^{-i\int_0^\Lambda d\lambda \boldsymbol{A}_{\mathrm{U}}}. \tag{7}$$

Here, $\mathcal{P}$ denotes path ordering, and $\boldsymbol{A}_{\mathrm{U}} = i\partial_\lambda \mathsf{U}(\lambda)\mathsf{U}^\dagger(\lambda)$ is the U(n) Uhlmann connection. The U(n) gauge freedom can be reduced to U(1) by performing a trace which leads to the Uhlmann phase

$$\phi^{\mathrm{U}} = \mathrm{Im}\ln \mathrm{Tr}[\rho(0)\mathcal{H}_{\mathrm{U}}]. \tag{8}$$

For (pure) ground states of gapped fermionic models, Eq. (8) reduces to the well-known Zak phase, if λ is identified with the lattice momentum k.

In Ref. [12], the winding of the Uhlmann phase (8) upon a cyclic change in an external parameter t was proposed as a topological invariant to classify one-dimensional lattice models in a mixed state ρ:

$$\nu^{\mathrm{U}} = \frac{1}{2\pi} \int_0^T dt\, \frac{\partial}{\partial t} \phi^{\mathrm{U}}(t). \tag{9}$$

Here, the variable λ entering the definition of the Uhlmann phase is the quasimomentum k along the chain, and the loop integral extends over the first Brillouin zone $\{\lambda \to k \in [-\pi, \pi)\}$. While this defines a consistent invariant in one dimension, its extension to two spatial dimensions as proposed in Refs. [13,14] is problematic. As shown by Budich and Diehl [16], the windings of the Uhlmann phase in the x or y direction are in general not the same, i.e.,

$$\begin{aligned}C^{\mathrm{U}}_x &= \frac{1}{2\pi} \oint_{\mathrm{BZ}} dk_y \frac{\partial}{\partial k_y} \phi^{\mathrm{U}}_x(k_y) \\ &\neq -\frac{1}{2\pi} \oint_{\mathrm{BZ}} dk_x \frac{\partial}{\partial k_x} \phi^{\mathrm{U}}_y(k_x) = C^{\mathrm{U}}_y.\end{aligned} \tag{10}$$

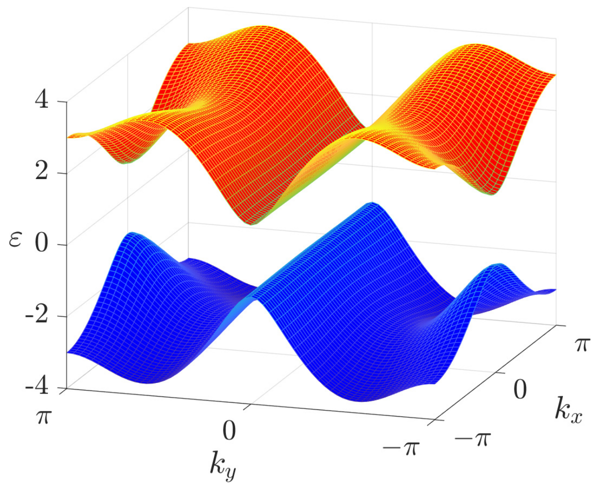

FIG. 1. Spectrum of asymmetric Qi-Wu-Zhang model.

As an example they considered a finite-temperature state of a simple topological two-band model with asymmetric band structure

$$\hat{\mathcal{H}}(\boldsymbol{k}) = \boldsymbol{d}(\boldsymbol{k}) \cdot \boldsymbol{\sigma} = \sum_{j=1}^{3} d_j(\boldsymbol{k})\, \sigma_j, \tag{11}$$

$$\boldsymbol{d}(\boldsymbol{k}) = \begin{pmatrix} \sin(k_x) \\ 3\sin(k_y) \\ 1-\cos(k_x)-\cos(k_y) \end{pmatrix}, \tag{12}$$

which is a modification of the Qi-Wu-Zhang model [28]. Here, $\boldsymbol{\sigma}$ is the vector of the Pauli matrices. Its band spectrum is shown in Fig. 1. While at temperatures $T=0$ or $T=\infty$ the windings of the Uhlmann phase in both directions are the same, i.e., $C_y^{\mathrm{U}}(T=0) = C_x^{\mathrm{U}}(T=0) = 1$ and $C_y^{\mathrm{U}}(T=\infty) = C_x^{\mathrm{U}}(T=\infty) = 0$, there is a range of temperatures where $C_y^{\mathrm{U}}(T) \neq C_x^{\mathrm{U}}(T)$. This shows that in contrast to the full $\mathrm{U}(n)$ Uhlmann holonomy, there is no proper U(1) gauge structure underlying the Uhlmann phase.

IV. MANY-BODY POLARIZATION AND ENSEMBLE GEOMETRIC PHASE

In the following we want to show that in contrast to the Uhlmann phase, the ensemble geometric phase, introduced for one-dimensional lattice models in Refs. [17,18], can be used to define a proper Berry curvature and Chern number for mixed states of 2D band structures.

A. Ground-state Zak phase and many-body polarization

A physical interpretation of the Zak phase can be picked up from its relation to the many-body polarization of insulating states, which in the form introduced by Resta [25] reads

$$P = \frac{1}{2\pi} \mathrm{Im} \ln \langle e^{\frac{2\pi i}{N}\hat{X}} \rangle. \tag{13}$$

Here, $\hat{X} = \sum_{j=1}^{N} \sum_{\lambda=1}^{p} j \hat{n}_{j;\lambda}$ is the position operator of all particles, and the average is performed with respect to the insulating many-body ground state $|\Psi_0\rangle$. Here, $\hat{n}_{j;\lambda} = \hat{c}_{j;\lambda}^{\dagger} \hat{c}_{j;\lambda}$ is the number operator of fermions in the λth site of the jth unit cell in a periodic system of size $L = pN$. We have disregarded the relative position of sites within the unit cell. The latter can straightforwardly be incorporated but does not affect the key properties of P. One immediately recognizes that the many-body polarization is the phase of a complex number, given by the expectation value of the collective momentum shift operator $e^{\frac{2\pi i}{N}\hat{X}}$ divided by 2π. In fact, as shown by King-Smith and Vanderbilt [29], differences in P are strictly related to differences in the Zak phase via

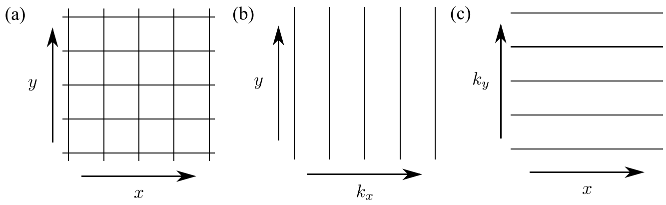

FIG. 2. The Chern number of a two-dimensional, translational invariant lattice model (a) can be represented as the winding of Zak phases of one-dimensional chains. This can be done in two different ways, either by the winding of the Zak phase $\phi_y = \phi_x(k_x)$ upon cyclic changes in the lattice momentum k_x (b) or by the (negative) winding of the Zak phase $\phi_x = \phi_x(k_y)$ upon cyclic changes in k_y (c).

$$\Delta P = \frac{1}{2\pi} \Delta\phi^{\mathrm{Zak}}. \tag{14}$$

If the system Hamiltonian is time dependent with period T, the polarization becomes time dependent as well and its winding upon adiabatic changes in a period $(0, T)$ is the Chern number of a Berry connection on a 2D torus (k, t) of lattice momentum and time

$$C = \frac{i}{2\pi} \int_0^T dt \oint_{\mathrm{BZ}} dk\, \langle \partial_t u(k) | \partial_k u(k) \rangle. \tag{15}$$

For translationally invariant 2D models, one can introduce a polarization vector by mapping the 2D system to a set of independent 1D chains in either the x or y direction; see Fig. 2:

$$P_x(k_y) = \frac{1}{2\pi} \mathrm{Im} \ln \left\langle e^{\frac{2\pi i}{N}\hat{X}(k_y)} \right\rangle, \tag{16}$$

$$P_y(k_x) = \frac{1}{2\pi} \mathrm{Im} \ln \left\langle e^{\frac{2\pi i}{N}\hat{Y}(k_x)} \right\rangle, \tag{17}$$

with $\hat{X}(k_y) = \sum_{j_x=1}^{N} \sum_{\lambda=1}^{p} j_x \hat{c}_{j_x,\lambda}^{\dagger}(k_y) \hat{c}_{j_x,\lambda}(k_y)$, where $\hat{c}_{j_x,\lambda}(k_y)$ is the fermion annihilation operator in mixed position-momentum space. Similarly, $\hat{Y}(k_x) = \sum_{j_y=1}^{N} \sum_{\lambda=1}^{p} j_y \hat{c}_{j_y,\lambda}^{\dagger}(k_x) \hat{c}_{j_y,\lambda}(k_x)$. Applying the King-Smith–Vanderbilt relations to the individual components of the polarization vector

$$\Delta P_x(k_y) = \frac{1}{2\pi} \Delta\phi_x^{\mathrm{Zak}}(k_y), \qquad \Delta P_y(k_x) = \frac{1}{2\pi} \Delta\phi_y^{\mathrm{Zak}}(k_x)$$

and taking into account Eq. (5) shows that there are two equivalent representations of the lattice Chern number in the gapped ground state in terms of polarization components

$$C_0 = \oint_{\mathrm{BZ}} dk_y \frac{\partial}{\partial k_y} P_x(k_y) \Big|_{\Psi_0} = -\oint_{\mathrm{BZ}} dk_x \frac{\partial}{\partial k_x} P_y(k_x) \Big|_{\Psi_0}. \tag{18}$$

B. Ensemble geometric phase

In contrast to the Zak phase, which has a meaning only for pure states, the many-body polarization can also be evaluated if the system is in a mixed state ρ. This then defines the ensemble geometric phase (EGP):

$$\phi^{\mathrm{EGP}} = \mathrm{Im} \ln \mathrm{Tr}\big\{\rho\, e^{\frac{2\pi i}{N}\hat{X}}\big\}. \tag{19}$$

The EGP was introduced in Refs. [17,18] as an alternative to the Uhlmann phase for the definition of topological invariants in 1D lattices. Considering the change in the EGP upon an adiabatic, closed loop in parameter space leads to an integer-valued winding number, which is a topological invariant as long as certain generalized gap conditions are fulfilled [18]. Note that while the EGP is equally applicable to boson systems, mixed states of noninteracting bosons always lead to trivial winding numbers due to the lack of Pauli exclusion [30]. The EGP can be measured [18], and its nontrivial winding has direct physical implications such as quantized transport in a weakly coupled auxiliary system [26].

C. Berry curvature and Chern number for Gaussian mixed states

We here consider a special class of mixed states, Gaussian states, which are the analog of pure many-body eigenstates of noninteracting fermions. Gaussian states of translationally invariant systems can always be written in the form

$$\rho = \frac{1}{Z}\exp\left\{-\sum_{\boldsymbol{k}} \tilde{\mathbf{c}}^\dagger(\boldsymbol{k})\mathsf{g}(\boldsymbol{k})\tilde{\mathbf{c}}(\boldsymbol{k})\right\} \tag{20}$$

and are fully determined by a $p\times p$ Hermitian matrix $\mathsf{g}(\boldsymbol{k})$. Note that we have restricted ourselves for simplicity to systems with particle number conservation. Here, $\boldsymbol{k} = (k_x, k_y)$ is the lattice momentum vector, and we used the abbreviation $\tilde{\mathbf{c}}(\boldsymbol{k}) = (\tilde{c}_1(\boldsymbol{k}), \dots, \tilde{c}_p(\boldsymbol{k}))$. g is directly related to the covariance matrix of single-particle correlations

$$\mathsf{h}^{\mathrm{fict}}_{\mu\nu}(\boldsymbol{k}) = \langle \tilde{c}^\dagger_\mu(\boldsymbol{k})\tilde{c}_\nu(\boldsymbol{k})\rangle = \frac{1}{2}\left[1-\tanh\left(\frac{\mathsf{g}(\boldsymbol{k})}{2}\right)\right]_{\nu,\mu}, \tag{21}$$

which was termed a *fictitious Hamiltonian* in Ref. [11]. Equation (20) has the form of a grand-canonical density matrix, and indeed for a finite-temperature state one finds

$$\mathsf{g}(\boldsymbol{k}) = \beta(\mathsf{h}(\boldsymbol{k}) - \mu), \tag{22}$$

where $\mathsf{h}(\boldsymbol{k})$ is the (original) single-particle Hamiltonian, $\beta = 1/(k_B T)$, and μ is the chemical potential.

While all results can be applied to genuine nonequilibrium, Gaussian steady states, we will focus in the following on finite-temperature states. In this context it is important to note that all single-particle Bloch states of the original Hamiltonian $\mathsf{h}(\boldsymbol{k})$ and those of $\mathsf{h}^{\mathrm{fict}}(\boldsymbol{k})$ are the same and thus all topological properties carry over. Viewing the fictitious Hamiltonian as the central quantity of Gaussian mixed states also implies that it determines their topological classification following the Altland-Zirnbauer scheme [31–33] with ten distinct symmetry classes. One further concludes that a topological phase transition can take place when the gap of $\mathsf{h}^{\mathrm{fict}}$ closes. For thermal states this can happen either if the gap of the original Hamiltonian h closes or if $\beta \to 0$. Thus the critical temperature of a topological phase transition of the fictitious Hamiltonian is always $T_c = \infty$ irrespective of the details of h as long as it remains gapped. This is a crucial difference compared with the Uhlmann phase, where for several examples a *finite* critical temperature was found [12,14].

If we consider an equilibrium state where the chemical potential is within a band gap of h, also $\mathsf{h}^{\mathrm{fict}}$ has an energy gap which is centered around zero "energy." It was shown in Ref. [18] that for 1D band structures the EGP then reduces in the thermodynamic limit to the Zak phase of the many-body ground state $|\Psi_0\rangle$ of the fictitious Hamiltonian via a mechanism termed gauge reduction:

$$\phi^{\mathrm{EGP}}(\rho) = \phi^{\mathrm{Zak}}(|\Psi_0\rangle\langle\Psi_0|) + O(N^{-\alpha}), \tag{23}$$

with some $\alpha > 0$. Furthermore, since the winding of ϕ^{EGP} as well as that of ϕ^{Zak} upon an adiabatic parameter loop must be a multiple of 2π, the winding numbers for any system size N are equal, $\nu^{\mathrm{Zak}}|_{\Psi_0} = \nu^{\mathrm{EGP}}|_\rho$, and

$$\begin{aligned}\nu^{\mathrm{EGP}}|_\rho &= \frac{1}{2\pi}\int_0^\Lambda d\lambda\, \frac{\partial}{\partial\lambda}\phi^{\mathrm{EGP}}\\ &= \frac{i}{2\pi}\int_0^\Lambda d\lambda \oint_{\mathrm{BZ}} dk\,(\langle\partial_\lambda u_f(k)|\partial_k u_f(k)\rangle - \mathrm{c.c.}),\end{aligned} \tag{24}$$

where $|u_f(k)\rangle$ are the Bloch states of the negative energy bands of the fictitious Hamiltonian.

$$\mathsf{h}^{\mathrm{fict}}(k)\,|u_f^{(n)}(k)\rangle = \varepsilon_n(k)\,|u_f^{(n)}(k)\rangle. \tag{25}$$

We note that while for thermal states the Bloch wave functions of $\mathsf{h}^{\mathrm{fict}}$ are just those of the original Hamiltonian h, the $|u_f(k)\rangle$'s have a meaning of their own in the case of a nonequilibrium steady state.

We now argue that the same is true for a finite-temperature state in two spatial dimensions, if the system is translationally invariant, i.e., if a decomposition in independent one-dimensional systems such as those shown in Fig. 2 is possible. In such a case the density matrix at nonzero temperature can be decomposed in two different ways:

$$\begin{aligned}\rho &= \frac{1}{Z}\prod_{k_x}\exp\left\{-\sum_q \hat{\mathbf{c}}^\dagger(k_x,q)\,\mathsf{g}(k_x,q)\,\hat{\mathbf{c}}(k_x,q)\right\}\\ &= \frac{1}{Z}\prod_{k_y}\exp\left\{-\sum_q \hat{\mathbf{c}}^\dagger(q,k_y)\,\mathsf{g}(q,k_y)\,\hat{\mathbf{c}}(q,k_y)\right\}.\end{aligned} \tag{26}$$

Then, along the lines of Ref. [18] the winding of the ensemble geometric phase in the x or y direction upon moving k_y or k_x through the Brillouin zone is the same as that of the Zak phase in the ground state of the fictitious Hamiltonian

$$\begin{aligned}C_x^{\mathrm{EGP}} &= \frac{1}{2\pi}\oint_{\mathrm{BZ}} dk_y\, \frac{\partial}{\partial k_y}\phi_x^{\mathrm{EGP}}(k_y)\\ &= \frac{i}{2\pi}\oiint_{\mathrm{BZ}} dk_x\, dk_y\big(\langle\partial_{k_x}u_f(\boldsymbol{k})|\partial_{k_y}u_f(\boldsymbol{k})\rangle - \mathrm{c.c.}\big),\end{aligned} \tag{27}$$

$$\begin{aligned}C_y^{\mathrm{EGP}} &= -\frac{1}{2\pi}\oint_{\mathrm{BZ}} dk_x\, \frac{\partial}{\partial k_x}\phi_y^{\mathrm{EGP}}(k_x)\\ &= -\frac{i}{2\pi}\oiint_{\mathrm{BZ}} dk_x\, dk_y\big(\langle\partial_{k_y}u_f(\boldsymbol{k})|\partial_{k_x}u_f(\boldsymbol{k})\rangle - \mathrm{c.c.}\big).\end{aligned} \tag{28}$$

Obviously, both expressions are the same and can be written as an integral of a Berry curvature $\mathcal{F}^{\mathrm{EGP}}(\boldsymbol{k})$ over the two-dimensional Brillouin zone

$$C^{\mathrm{EGP}} = C_x^{\mathrm{EGP}} = C_y^{\mathrm{EGP}} = \frac{1}{2\pi} \oiint_{\mathrm{BZ}} d\boldsymbol{k}\, \mathcal{F}^{\mathrm{EGP}}(\boldsymbol{k}). \tag{29}$$

$\mathcal{F}^{\mathrm{EGP}}(\boldsymbol{k})$ is the Berry curvature of the ground state of the fictitious Hamiltonian

$$\begin{aligned}\mathcal{F}^{\mathrm{EGP}}(\boldsymbol{k}) &= (\nabla_k \times \boldsymbol{A}^{\mathrm{EGP}}(\boldsymbol{k}))_z \\ &= i(\langle \partial_{k_x} u_f(\boldsymbol{k}) | \partial_{k_y} u_f(\boldsymbol{k})\rangle - \langle \partial_{k_y} u_f(\boldsymbol{k}) | \partial_{k_x} u_f(\boldsymbol{k})\rangle).\end{aligned} \tag{30}$$

We conclude that for the two-dimensional generalization of the ensemble geometric phase there exists always a proper Berry curvature. The corresponding Chern number can be nonzero only if the fictitious Hamiltonian $\mathsf{h}^{\mathrm{fict}}(\boldsymbol{k})$ breaks time-reversal symmetry. For thermal states this is the case if the original Hamiltonian $\mathsf{h}(\boldsymbol{k})$ breaks time-reversal symmetry.

The reduction of topological properties of Gaussian mixed states of fermions in two dimensions to the ground state of the fictitious Hamiltonian is fully consistent with the general finding that there are only 10 symmetry classes to classify steady states of open systems rather than 28 as expected, for example, for non-Hermitian Hamiltonians [34,35].

To illustrate our findings, we calculated the EGP components of the asymmetric Qi-Wu-Zhang model, Eq. (3), for a finite-temperature state for a finite system of $N \times N$ unit cells. The results are shown in Fig. 3 for $T = 0$ and a temperature much above the single-particle energy gap $T = 20\Delta_{\mathrm{gap}}$. For the higher temperature we have also shown the results for different system sizes $N = 10, 50, 100$. One clearly recognizes the gauge reduction discussed in Ref. [18]: Even at a temperature much above the single-particle gap the EGP approaches the ground-state value for increasing N. Its winding, which determines the topological invariant, is furthermore independent of system size. Moreover, in contrast to the Uhlmann phase, the winding of both components ϕ_x^{EGP} and $-\phi_y^{\mathrm{EGP}}$ is always the same for all finite temperatures $T < \infty$.

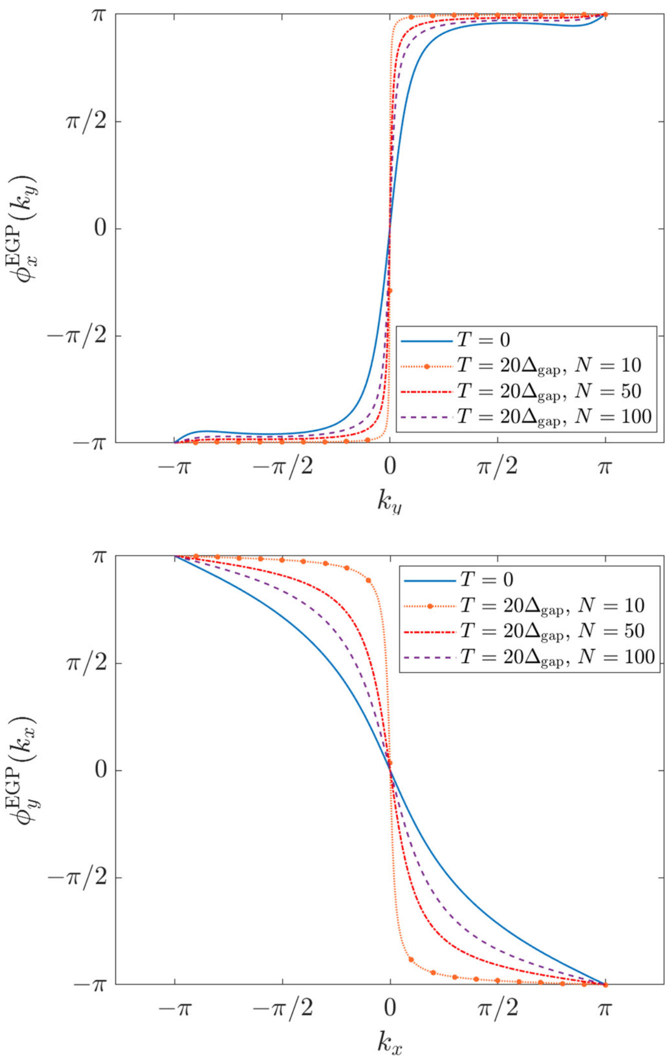

FIG. 3. EGP of the Qi-Wu-Zhang model in the x direction as a function of k_y (top) and in the y direction as a function of k_x (bottom) for different temperatures. One recognizes that in contrast to the Uhlmann case, the windings of both are exactly the same (with the proper sign convention) for all temperatures even much above the single-particle gap.

V. SUMMARY

We have shown that the ensemble geometric phase which has been used to define topological winding numbers for mixed states of one-dimensional, Gaussian fermion systems can straightforwardly be extended to two spatial dimensions and defines a Chern number if there is translational invariance. Different from approaches based on other geometric phases for mixed states, such as the Uhlmann phase, this number is a true topological invariant as it is a two-dimensional integral over a proper Berry curvature. The latter is defined by the Bloch states of the fictitious Hamiltonian formed by the matrix of single-particle correlations in the Gaussian mixed state. Finite-temperature states of noninteracting fermion models, which are fully characterized by single-particle correlations, are Gaussian, but Gaussian states can also emerge as nonequilibrium steady states of systems coupled to specific Markovian reservoirs. In the first case the mixed-state Berry curvature is identical to that of the original Bloch Hamiltonian counting all bands below the chemical potential as long as $T < \infty$. For genuine nonequilibrium states, no such correspondence exists, and the fictitious Hamiltonian has a meaning of its own. While the discussion in this paper relies on the assumption of translational invariance, allowing a mapping to decoupled one-dimensional chains (see Fig. 2), we anticipate the results to hold also in the presence of disorder and with interactions. Further studies are needed on this subject.

ACKNOWLEDGMENT

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