Uhlmann Phase as a Topological Measure for One-Dimensional Fermion Systems

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We introduce the Uhlmann geometric phase as a tool to characterize symmetry-protected topological phases in one-dimensional fermion systems, such as topological insulators and superconductors. Since this phase is formulated for general mixed quantum states, it provides a way to extend topological properties to finite temperature situations. We illustrate these ideas with some paradigmatic models and find that there exists a critical temperature T_c at which the Uhlmann phase goes discontinuously and abruptly to zero. This stands as a borderline between two different topological phases as a function of the temperature. Furthermore, at small temperatures we recover the usual notion of topological phase in fermion systems.

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Introduction.—Geometric phases have played an essential role in many quantum phenomena since their modern discovery by Berry [1] (see also Refs. [2,3]). An emblematic example is the characterization of the transversal conductivity σ_{xy} in the quantum Hall effect by means of the integral of the Berry curvature over the two-dimensional Brillouin zone (BZ), in units of e^2/h. This is the celebrated TKNN formula [4] that has become a key ingredient in the characterization in the newly emerging field of topological insulators [5,6]. Recently, the experimental measurement of a Berry phase in a one-dimensional optical lattice (Zak phase [7]) simulating the different phases of polyacetylene [8] has opened the way to extend the applications of geometric phases to study topological properties beyond the realm of condensed-matter systems.

A fundamental problem in the theory and applications of geometrical phases is its extension from pure quantum states (Berry) to mixed quantum states described by density matrices. Uhlmann was the first to mathematically address this issue [9] and to provide a satisfactory solution [10–13]. For more than a decade, there has been a renewed interest in studying geometric phases for mixed states and under dissipative evolutions from the point of view of quantum information [14], and more inequivalent definitions have been introduced [15–17]. This has culminated with the first experimental measurement of a geometric phase for mixed quantum states of one system qubit and one ancillary qubit with NMR techniques [18].

In addition, the role played by external dissipative effects and thermal baths in topological insulators and superconductors has attracted much interest both in quantum simulations with different platforms and in condensed matter [19–29]. In this Letter, we show that the Uhlmann geometric phase is endowed with a topological structure when applied to one-dimensional fermion systems. More concretely, (i) we show that the Uhlmann phase allows us to characterize topological insulators and superconductors at both zero and finite temperatures. (ii) We find a finite critical temperature T_c below which the Uhlmann phase is constant and nonvanishing. At T_c there is a discontinuity, and above it the topological behavior ceases to exist. This kind of behavior is very relevant and not present in other formulations. (iii) We study one-dimensional (1D) paradigmatic models such as the Creutz ladder (CL) [30,31], the Majorana chain (MC) [32], and polyacetylene (SSH) [33,34]. A summary of the basic results of this Letter is presented in Table I. Notably, at the limit of zero temperature the Uhlmann phase recovers the usual notion of topological order as given by the Berry phase. Moreover, when the three models are in a flat-band regime the critical temperature is universal [Eq. (15)].

The Uhlmann approach is based on the concept of amplitude. An amplitude for some density matrix ρ is any of the matrices w such that

$$\rho = ww^\dagger. \tag{1}$$

The key idea behind this definition is that the amplitudes form a Hilbert space $\mathcal{H}_w$ with the Hilbert-Schmidt product $(w_1, w_2) := \mathrm{Tr}(w_1^\dagger w_2)$. On the contrary, the set of density matrices $\mathcal{Q}$ is not a linear space. From Eq. (1), we see that there is a $\mathrm{U}(n)$-gauge freedom in the choice of the amplitude (n is the dimension of the space): w and wU are amplitudes of the same state for some unitary operator U.

TABLE I. Comparison of Hamiltonian winding number, Berry, and Uhlmann phases for nontrivial topological regimes in the Creutz ladder (CL), Majorana chain (MC), and polyacetylene (SSH) 1D fermion models.

Topological measures in 1D fermion models	CL	MC	SSH
Winding number ($T=0$)	1	1	1
Berry phase ($T=0$)	π	π	π
Uhlmann phase ($T<T_c$)	π	π	π
Uhlmann phase ($T>T_c$)	0	0	0

Note the parallelism with the usual U(1)-gauge freedom of pure states, where $|\psi\rangle$ and $e^{i\phi}|\psi\rangle$ represent the same physical state, i.e., the same density matrix given by $|\psi\rangle\langle\psi|$. Thus, the usual gauge freedom can be seen as a particular case of the amplitude U(n)-gauge freedom.

An amplitude is nothing but another way to see the concept of purification. Indeed, by the polar decomposition theorem, we parametrize the possible amplitudes of some density matrix ρ as $w=\sqrt{\rho}U$. Because of the spectral theorem $\rho=\sum_j p_j|\psi_j\rangle\langle\psi_j|$, we have $w=\sum_j\sqrt{p_j}|\psi_j\rangle\langle\psi_j|U$. Let us define the following isomorphism between the spaces $\mathcal{H}_w$ and $\mathcal{H}\otimes\mathcal{H}$: $w=\sum_j\sqrt{p_j}\,|\psi_j\rangle\langle\psi_j|U\longleftrightarrow|w\rangle=\sum_j\sqrt{p_j}\,|\psi_j\rangle\otimes U^{\mathrm{t}}|\psi_j\rangle$ (here the transposition is taken with respect to the eigenbasis of ρ). The property $\rho=ww^\dagger$ is now written as

$$\rho=\mathrm{Tr}_2(|w\rangle\langle w|). \tag{2}$$

Here, Tr_2 denotes the partial trace over the second Hilbert space of $\mathcal{H}\otimes\mathcal{H}$. In other words, any amplitude w of some density matrix ρ can be seen as a pure state $|w\rangle$ of the enlarged space $\mathcal{H}\otimes\mathcal{H}$, with partial trace equal to ρ. Thus, $|w\rangle$ is a purification of ρ.

Let us consider a family of pure states $|\psi_{\boldsymbol{k}}\rangle\langle\psi_{\boldsymbol{k}}|$ and some trajectory in parameter space $\{\boldsymbol{k}(t)\}_{t=0}^1$, such that the initial and final states are the same. This induces a trajectory on the Hilbert space $\mathcal{H}$, $|\psi_{\boldsymbol{k}(t)}\rangle$, and since the path on $\mathcal{Q}$ is closed, the initial and final vectors are equivalent up to some Φ, $|\psi_{\boldsymbol{k}(1)}\rangle=e^{i\Phi}|\psi_{\boldsymbol{k}(0)}\rangle$. Provided the transportation of the vectors in $\mathcal{H}$ is done following the Berry parallel transport condition (i.e., no dynamical phase is accumulated) Φ is the well-known Berry phase Φ_B. This depends only on the geometry of the path and can be written as $\Phi_B=\oint A_B$, where $A_B:=i\sum_\mu\langle\psi_{\boldsymbol{k}}|\partial_\mu\psi_{\boldsymbol{k}}\rangle dk_\mu$ is the Berry connection form ($\partial_\mu:=\partial/\partial k_\mu$). Similarly, we may have a closed trajectory of not necessarily pure density matrices $\rho_{\boldsymbol{k}}$, which in turn induces a trajectory on the Hilbert space $\mathcal{H}_w$, $w_{\boldsymbol{k}(t)}$. Again, since the path on $\mathcal{Q}$ is closed, the initial and final amplitudes must differ just in some unitary transformation V, $w_{\boldsymbol{k}(1)}=w_{\boldsymbol{k}(0)}V$. Hence, by analogy to the pure state case, Uhlmann defines a parallel transport condition such that V is given by $V=\mathcal{P}e^{\oint A_U}U_0$, where $\mathcal{P}$ stands for the path ordering operator, A_U is the Uhlmann connection form, and U_0 is the gauge taken at $\boldsymbol{k}(0)$. We have illustrated this parallelism between the Berry and Uhlmann approaches in Fig. 1.

The Uhlmann parallel transport condition asserts that for some point $\rho_{\boldsymbol{k}(t)}$ with amplitude $w_{\boldsymbol{k}(t)}$ the amplitude $w_{\boldsymbol{k}(t+dt)}$ of the next point in the trajectory, $\rho_{\boldsymbol{k}(t+dt)}$, is the closest [35] to $w_{\boldsymbol{k}(t)}$ among the possible amplitudes of $\rho_{\boldsymbol{k}(t+dt)}$. With this rule, it is possible to obtain some explicit formulas for A_U. Concretely, in the spectral basis of $\rho_{\boldsymbol{k}}=\sum_j p_{\boldsymbol{k}}^j|\psi_{\boldsymbol{k}}^j\rangle\langle\psi_{\boldsymbol{k}}^j|$, one obtains [12]

$$A_U=\sum_{\mu,i,j}|\psi_{\boldsymbol{k}}^i\rangle\frac{\langle\psi_{\boldsymbol{k}}^i|[(\partial_\mu\sqrt{\rho_{\boldsymbol{k}}}),\sqrt{\rho_{\boldsymbol{k}}}]|\psi_{\boldsymbol{k}}^j\rangle}{p_{\boldsymbol{k}}^i+p_{\boldsymbol{k}}^j}\langle\psi_{\boldsymbol{k}}^j|dk_\mu. \tag{3}$$

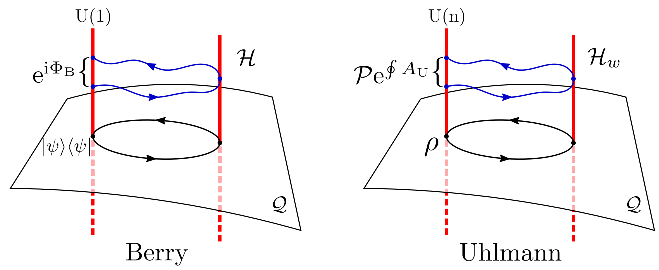

FIG. 1 (color online). Comparison of the Berry and Uhlmann approaches. The usual U(1)-gauge freedom is generalized to the $U(n)$-gauge freedom of the amplitudes in the Uhlmann approach. Thus, according to Berry, after a closed loop in the set $\mathcal{Q}$, a pure state carries a simple phase factor Φ_B. However, for mixed states, the amplitude carries a unitary matrix $\mathcal{P}e^{\oint A_U}$.

Note that this connection form has only zeroes on its diagonal and is skew adjoint so that the Uhlmann connection is special unitary. The Uhlmann geometric phase along a closed trajectory $\{\boldsymbol{k}(t)\}_{t=0}^1$ is defined as

$$\Phi_U:=\arg\langle w_{\boldsymbol{k}(0)}|w_{\boldsymbol{k}(1)}\rangle=\arg\mathrm{Tr}[w_{\boldsymbol{k}(0)}^\dagger w_{\boldsymbol{k}(1)}]. \tag{4}$$

By the polar decomposition theorem, we may write $w_{\boldsymbol{k}(0)}=\sqrt{\rho_{\boldsymbol{k}(0)}}U_0$, $w_{\boldsymbol{k}(1)}=\sqrt{\rho_{\boldsymbol{k}(0)}}V$, so that

$$\Phi_U=\arg\mathrm{Tr}[\rho_{\boldsymbol{k}(0)}\mathcal{P}e^{\oint A_U}]. \tag{5}$$

As aforementioned, in this work we shall focus on the Uhlmann phase in 1D fermion models. For such systems, $\boldsymbol{k}\equiv k$ is the one-dimensional crystalline momentum living in a S^1-circle BZ. Thus, because of the nontrivial topology of S^1, geometric phases after a loop in k acquire a topological sense.

Fermionic systems and Uhlmann phase.—Consider two-band Hamiltonians within the spinor representation $\Psi_k=(\hat{a}_k,\hat{b}_k)^{\mathrm{t}}$, where $\hat{a}_k$ and $\hat{b}_k$ stands for two species of fermionic operators. For superconductors, the spinor Ψ_k is constructed out of a Nambu transformation of paired fermions with opposite crystalline momentum [36]. The Hamiltonian is a quadratic form $H=\sum_k\Psi_k^\dagger H_k\Psi_k$, and H_k is a 2×2 matrix

$$H_k=f(k)\mathbb{1}+\frac{\Delta_k}{2}\boldsymbol{n}_k\cdot\boldsymbol{\sigma}. \tag{6}$$

Here, $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ are the Pauli matrices, Δ_k corresponds to the gap of H_k, and $f(k)$ denotes some function of k. The unit vector $\boldsymbol{n}_k=(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)$ is called the "winding vector" where θ and ϕ are k-dependent spherical coordinates. The band eigenvectors of H_k can be written as

$$|u_-^k\rangle=\begin{pmatrix}-e^{-i\phi(k)}\sin\frac{\theta(k)}{2}\\ \cos\frac{\theta(k)}{2}\end{pmatrix},\qquad|u_+^k\rangle=\begin{pmatrix}e^{-i\phi(k)}\cos\frac{\theta(k)}{2}\\ \sin\frac{\theta(k)}{2}\end{pmatrix}. \tag{7}$$

If the thermalization process preserves particle number and the Fermi energy is set in the middle of the gap, the equilibrium (thermal) state is given by $\rho_\beta = \prod_k \rho_k^\beta$, with

$$\rho_k^\beta = \frac{e^{-H_k/T}}{\mathrm{Tr}(e^{-H_k/T})} = \frac{1}{2}\left[\mathbb{1} - \tanh\left(\frac{\Delta_k}{2T}\right)\hat{\boldsymbol{n}}_k\cdot\boldsymbol{\sigma}\right], \quad (8)$$

where $T = 1/\beta$ denotes temperature.

By the use of Eq. (7), the Uhlmann connection (3) for ρ_k^β turns out to be

$$A_U^k = m_{12}^k \langle u_-^k|\partial_k u_+^k\rangle |u_-^k\rangle\langle u_+^k| dk + \mathrm{H.c.} \quad (9)$$

where $m_{12}^k := 1 - \mathrm{sech}[\Delta_k/(2T)]$.

Besides, it is well known that discrete symmetries represent a way to classify topological insulators and superconductors [37,38]. Furthermore, for the models considered throughout this Letter, symmetries impose a restriction on the movement of $\boldsymbol{n}_k$ to some plane as a function of k, making only two of its components n_k^i and n_k^j with $i \neq j$ different from zero. Therefore, we have a nontrivial mapping $S^1 \longrightarrow S^1$, characterized by a winding number ω_1. This is defined using the angle α covered by $\boldsymbol{n}_k$ when it winds around the unit circle S^1 and takes the form

$$\omega_1 := \frac{1}{2\pi}\oint d\alpha = \frac{1}{2\pi}\oint\left(\frac{\partial_k n_k^i}{n_k^j}\right)dk, \quad (10)$$

where we have used that $\alpha := \arctan(n_k^i/n_k^j)$.

Moreover, using Eqs. (7) and (10) with (9) and simplifying Eq. (5) we obtain an expression for the Uhlmann phase in terms of ω_1, the temperature, and parameters of the Hamiltonian

$$\Phi_U = \arg\left\{\cos(\pi\omega_1)\cos\left[\oint\left(\frac{\partial_k n_k^i}{2n_k^j}\right)\mathrm{sech}\left(\frac{\Delta_k}{2T}\right)dk\right]\right\}. \quad (11)$$

Particularly, in the limit $T \to 0$,

$$\Phi_U^0 = \arg[\cos(\pi\omega_1)]. \quad (12)$$

Note that for the trivial case $\omega_1 = 0$, the Uhlmann phase is zero as well. However, for nontrivial topological regions $\omega_1 = \pm 1$, we obtain $\Phi_U^0 = \pi$. Thus, the topological order as accounted by Φ_U^0 coincides to the standard notion measured by ω_1. In the following, we compute Φ_U at finite temperature for the three aforementioned models of topological insulators and superconductors.

Creutz ladder.—This model [30] is representative for a topological insulator [24,31] with AIII symmetry [37,38]. It describes the dynamics of spinless electrons moving in a ladder as dictated by the following Hamiltonian:

$$H_{\mathrm{CL}} = -\sum_{n=1}^{L}[R(e^{-i\Theta}a_{n+1}^\dagger a_n + e^{i\Theta}b_{n+1}^\dagger b_n) + R(b_{n+1}^\dagger a_n + a_{n+1}^\dagger b_n) + M a_n^\dagger b_n + \mathrm{H.c.}], \quad (13)$$

where a_n and b_n are fermionic operators associated to the nth site of an upper and lower chain, respectively. The hopping along horizontal and diagonal links is given by $R > 0$ and the vertical one by $M > 0$. In addition, a magnetic flux $\Theta \in [-\pi/2, \pi/2]$ is induced by a perpendicular magnetic field. For nonzero magnetic flux $\Theta \neq 0$ and small vertical hopping $m := M/2R < 1$, the system has localized edge states at the two ends of the open ladder [30]. Interestingly, there exists an experimental proposal for this model with optical lattices [39].

In momentum space, H_{CL} can be written in the form of Eq. (6) with (in units of $2R = 1$)

$$\boldsymbol{n}_k = \frac{2}{\Delta_k}(m + \cos k, 0, \sin\Theta\sin k),$$
$$\Delta_k = 2\sqrt{(m+\cos k)^2 + \sin^2\Theta\sin^2 k}, \quad (14)$$

which in the spinor decomposition made in Eq. (6) implies $\phi = 0, \pi$.

By the means of Eq. (11) we compute the value of the Uhlmann phase (which can only be equal to π or 0) as function of parameters Θ, m, and the temperature T [see Fig. 2(a)]. At $T \to 0$, the topological region coincides with the usual topological phase $\Phi_U^0 = \Phi_B = \pi$ for $m \in [0, 1]$ and $\Theta \in [-(\pi/2), (\pi/2)]$, as expected. However, there exists a critical temperature T_c for any value of the parameters at which the system is not topological in the Uhlmann sense anymore, and Φ_U goes abruptly to zero. The physical meaning of this T_c relies on the existence of some critical momentum k_c splitting the holonomy into two disequivalent topological components according to the value taken by k when performing the closed loop, $\Phi_U(k < k_c) = 0$ and $\Phi_U(k > k_c) = \pi$, respectively. In the trivial topological regime, there is only one component with $\Phi_U = 0$ for every point along the trajectory. Thus, this structure of the Uhlmann amplitudes accounts for a topological kink [40] in the holonomy along the BZ. Further details about the presence or absence with temperature of this topological kink can be seen in the Supplemental Material [41].

Interestingly, at $m = 0$ and $\Theta = \pm(\pi/2)$ (see the arrows in Fig. 2), the edge states become completely decoupled from the system dynamics. When considering periodic boundary conditions, this translates into having *flat bands* in the spectrum. For these flat-band points (FBPs) the critical temperature T_c only depends on the constant value of the gap $\Delta_k = 2$ and can be analytically computed. The result is the same for the three models analyzed in this work,

$$T_c = \frac{1}{\ln(2+\sqrt{3})}, \quad (15)$$

which is approximately 38% of the gap.

Majorana chain.—Consider a model of spinless fermions with p-wave superconducting pairing, hopping on

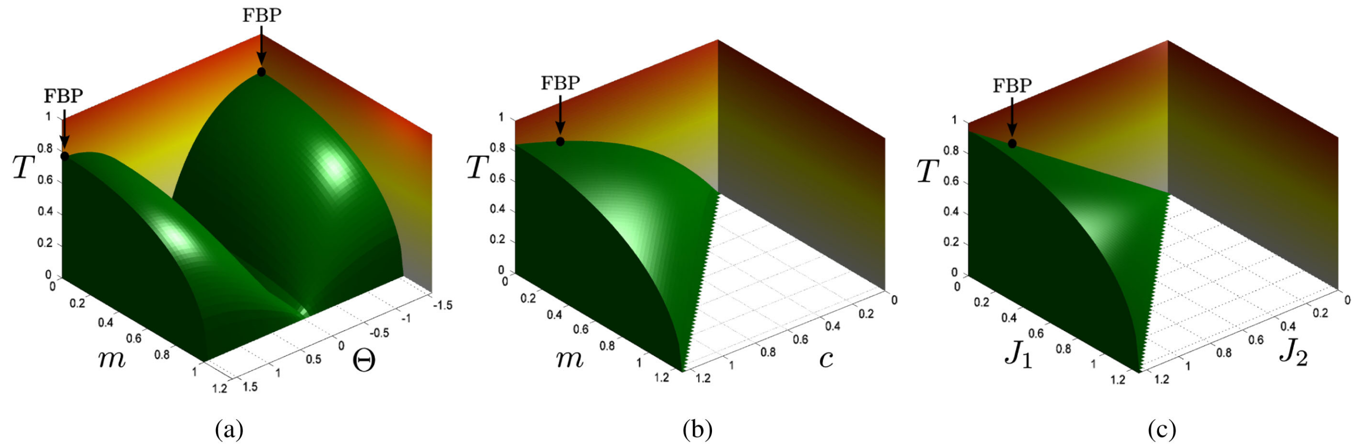

FIG. 2 (color online). Uhlmann topological phases for the CL (a), MC (b), and SSH (c). They are π inside the green volume and zero outside. The FBPs are indicated with an arrow and are universal. Natural units have been taken. In addition, for the CL and the MC we have fixed the horizontal hopping $2R = 1$ and the superconducting pairing $|M| = 1$, respectively.

an L-site one-dimensional chain. The Hamiltonian of this system introduced by Kitaev [32] is

$$H_{\mathrm{MC}} = \sum_{j=1}^{L}\left(-Ja_j^\dagger a_{j+1} + Ma_j a_{j+1} - \frac{\mu}{2}a_j^\dagger a_j + \mathrm{H.c.}\right), \tag{16}$$

where $\mu > 0$ is the chemical potential, $J > 0$ is the hopping amplitude, the absolute value of $M = |M|\mathrm{e}^{i\Theta}$ stands for the superconducting gap, and a_j $(a_j^\dagger)$ are annihilation (creation) fermionic operators.

For convenience, we may redefine new parameters $m := \mu/(2|M|)$ and $c := J/|M|$ and take $\Theta = 0$. It can be shown [32] that the system has nonlocal Majorana modes at the two ends on the chain if $m < c$, which corresponds to nonvanishing ω_1 and Φ_B when taking periodic boundary conditions. Thus, in momentum space, H_{MC} can be written in the form of Eq. (6) using the so-called Nambu spinors $\Psi_k = (a_k, a_{-k}^\dagger)^{\mathrm{t}}$,

$$\boldsymbol{n}_k = \frac{2}{\Delta_k}(0, -\sin k, -m + c\cos k),$$
$$\Delta_k = 2\sqrt{(-m + c\cos k)^2 + \sin^2 k}, \tag{17}$$

in units of $|M| = 1$. This in Eq. (6) implies $\phi = \pm(\pi/2)$.

In analogy to the CL case, we calculate the Uhlmann phase as a function of parameters m, c, and the temperature T [see Fig. 2(b)]. On the one hand, note again that at $T \to 0$ we recover the usual topological phase $\Phi_U^0 = \Phi_B = \pi$ for $m < c$, and on the other hand, there also exists a critical temperature T_c. The FBP corresponds to $m = 0$ and $c = 1$ where the Majorana modes are completely decoupled from the system dynamics. For the FBP, we get the same T_c as before (15) as shown in Fig. 2(b).

Polyacetylene (SSH model).—The following Hamiltonian was introduced in Ref. [34] by Rice and Mele, and it has a topological insulating phase

$$H_{\mathrm{SSH}} = -\sum_n (J_1 a_n^\dagger b_n + J_2 a_n^\dagger b_{n-1} + \mathrm{H.c.}) + M\sum_n (a_n^\dagger a_n - b_n^\dagger b_n). \tag{18}$$

The fermionic operators a_n and b_n act on adjacent sites of a dimerized chain. If the energy imbalance between sites a_n and b_n is $M = 0$, the above Hamiltonian $H \equiv H_{\mathrm{SSH}}$ effectively describes polyacetylene [33], whereas for $M \neq 0$ it can model diatomic polymers [34].

For $M = 0$ and $J_2 > J_1$, there are two edge states at the end of the chain and the system displays topological order, characterized by ω_1 and Φ_B.

In momentum space, H_{SSH} is written in the form of Eq. (6) with

$$\boldsymbol{n}_k = \frac{2}{\Delta_k}(-J_1 - J_2\cos k, J_2\sin k, 0),$$
$$\Delta_k = 2\sqrt{J_1^2 + J_2^2 + 2J_1J_2\cos k}, \tag{19}$$

which in Eq. (6) implies fixing $\theta = \pm(\pi/2)$ for all k.

In Fig. 2(c), we plot Φ_U as a function of the hopping parameters J_1, J_2, and the temperature T. At $T \to 0$, the topological region coincides again with the usual topological phase $\Phi_U^0 = \Phi_B = \pi$ for $J_1 < J_2$, and there exists a critical temperature T_c.

For the FBP, $J_1 = 0$ and $J_2 = 1$, the gap $\Delta_k = 2$ becomes constant and we obtain the same critical temperature as for the other two models; Eq. (15).

Outlook and conclusions.—We have shown that the Uhlmann phase provides us with a way to extend the notion of symmetry-protected topological order in fermion systems beyond the realm of pure states. This comes into play when studying dissipative effects and particularly thermal baths. When applied to three paradigmatic models of topological insulators and superconductors, it displays a discontinuity in some finite critical temperature T_c, which limits the region with topological behavior. Interestingly enough, a thermal-bulk-edge correspondence with the Uhlmann phase does not exist, and the topology assessed by it does not determine the fate of the edge modes at finite temperature.

Although the analysis has been restricted here to 1D models and some representative examples, we expect that the Uhlmann approach could be extended to higher spacial dimensions and other symmetry classes of topological insulators and superconductors. However, more progress on this line is required.

Finally, let us stress that the Uhlmann phase is an observable [42,43]. Additionally, we analyze possible experimental measurement schemes in the Supplemental Material [41].

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