Uhlmann Connection in Fermionic Systems Undergoing Phase Transitions

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We study the behavior of the Uhlmann connection in systems of fermions undergoing phase transitions. In particular, we analyze some of the paradigmatic cases of topological insulators and superconductors in one dimension, as well as the BCS theory of superconductivity in three dimensions. We show that the Uhlmann connection signals phase transitions in which the eigenbasis of the state of the system changes. Moreover, using the established fidelity approach and the study of the edge states, we show the absence of thermally driven phase transitions in the case of topological insulators and superconductors. We clarify what is the relevant parameter space associated with the Uhlmann connection so that it signals the existence of order in mixed states. In addition, the study of Majorana modes at finite temperature opens the possibility of applications in realistic stable quantum memories. Finally, the analysis of the different behavior of the BCS model and the Kitaev chain, with respect to the Uhlmann connection, suggested that in realistic scenarios the gap of topological superconductors could also, generically, be temperature dependent.

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Introduction.—Topological phases of matter have been a subject of active research during the last decades, as they constitute a whole new paradigm in condensed matter physics. In contrast to the well-studied standard quantum phases of matter, described by local order parameters (see, for example, Anderson's classification [1]), the ground states of topological systems are globally characterized by topological invariants [2–5]. Hamiltonians of gapped systems with different topological orders cannot be smoothly transformed from one into the other unless passing through a gap-vanishing region of criticality. In particular, insulators and superconductors with an energy gap exhibit topological orders and are classified according to the symmetries that their Hamiltonians possess [6,7], namely, time reversal, particle hole, and chiral symmetry. As opposed to the standard Landau symmetry breaking theory of quantum phase transitions (PTs), in topological PTs the symmetries of the Hamiltonian are not violated. For a topological PT to occur, that is a gapped state of the system to be deformed in another gapped state in a different topological class, the energy gap has to close. In other words, the quantum state of the system undergoing a topological PT is gapless. A manifestation of the topological order of a system is the presence of robust symmetry-protected edge states on the boundary between two distinct topological phases, as predicted by the bulk-to-boundary principle [8].

A question that naturally arises is whether there is any kind of topological order at finite temperatures, and different approaches have been used to tackle this problem [9,10]. One of the most promising approaches is based on the work of Uhlmann [11], who extended the notion of geometrical phases from pure states to density matrices. The concept of the Uhlmann holonomy, and the quantities that can be derived from it, were used to infer PTs at finite temperatures [12–17]. Nevertheless, the physical meaning of these quantities and their relevance to the observable properties of the corresponding systems stay as an interesting open question [18–20]. There exist several proposals for the observation of the Uhlmann geometric phase [21–23] and an experimental realization has been reported in Ref. [24].

Information-theoretic quantities such as entanglement measures [25–27] and the fidelity, a measure of distinguishability between two quantum states [28–32], were extensively used in the study of PTs. Whenever there is a PT, the density matrix of a system changes significantly and, therefore, a sudden drop of the fidelity $F(\rho,\sigma) \equiv \mathrm{Tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}$ signals out this change. The fidelity, is closely related to the Uhlmann connection, through the Bures metric [33]. Therefore, they can both be used to infer the possibility of PTs, as in Ref. [16] (for the pure-state case of the Berry phase, see Refs. [34,35]).

We analyze the behavior of the fidelity and the Uhlmann connection associated to thermal states in fermionic systems. We consider the space consisting of the parameters of the Hamiltonian and the temperature, as it provides a physically sensible base space for the principal bundle, describing the amplitudes of the density operator. We study paradigmatic models of 1D topological insulators (TIs) (Creutz Ladder [36,37] and Su-Schrieffer-Heeger [38] models) and superconductors (TSCs) (Kitaev chain [39]) with chiral symmetry. We conclude that the effective temperature only smears out the topological features exhibited at zero temperature, without causing a thermal PT. We also analyze the BCS model of superconductivity [40], previously studied in Ref. [16], by further identifying the significance of thermal and purely quantum contributions to PTs, using the fidelity and the Uhlmann connection. In contrast to the aforementioned nontrivial topological systems, both quantities indicate the existence of thermal PTs.

This Letter is organized as follows: first, we elaborate on the relationship between the fidelity and the Uhlmann connection and motivate their use in inferring PTs, both at zero and finite temperatures. In the following section, we present our results on the fidelity and the Uhlmann connection for the aforementioned systems and discuss the possibility of temperature driven PTs. In the last section we summarize our conclusions and point out possible directions of future work.

Fidelity and the Uhlmann parallel transport.—Given a Hilbert space, one can consider the set of density matrices with full rank (e.g., thermal states) and the associated set of amplitudes (generalization to the case of the sets of singular density matrices with fixed rank is straightforward). For a state ρ, an associated amplitude w satisfies $\rho = ww^\dagger$. Thus, there exists a unitary (gauge) freedom in the choice of the amplitude, since both w and $w' = wU$, with U being an arbitrary unitary, are associated to the same ρ. Two amplitudes w_1 and w_2, corresponding to states ρ_1 and ρ_2, respectively, are said to be *parallel* in the Uhlmann sense if and only if they minimize the Hilbert-Schmidt distance $\|w_1 - w_2\| = \sqrt{\mathrm{Tr}[(w_1 - w_2)^\dagger (w_1 - w_2)]}$, induced by the inner product $\langle w_1, w_2\rangle = \mathrm{Tr}(w_1^\dagger w_2)$. The condition of parallelism turns out to be equivalent to maximizing $\mathrm{Re}\langle w_1, w_2\rangle$, since $\|w_1 - w_2\|^2 = 2(1 - \mathrm{Re}\langle w_1, w_2\rangle)$. By writing $w_i = \sqrt{\rho_i}U_i$, $i = 1, 2$, where the U_i's are unitary matrices, we get

$$\begin{aligned}\mathrm{Re}\langle w_1,w_2\rangle \leq |\langle w_1,w_2\rangle| &= |\mathrm{Tr}(w_2^\dagger w_1)| \\ &= |\mathrm{Tr}(U_2^\dagger \sqrt{\rho_2}\sqrt{\rho_1}U_1)| \\ &= |\mathrm{Tr}(|\sqrt{\rho_2}\sqrt{\rho_1}|UU_1U_2^\dagger)| \\ &\leq \mathrm{Tr}(|\sqrt{\rho_2}\sqrt{\rho_1}|) \\ &= \mathrm{Tr}\sqrt{\sqrt{\rho_1}\rho_2\sqrt{\rho_1}} = F(\rho_1,\rho_2), \quad (1)\end{aligned}$$

where U is the unitary associated to the polar decomposition of $\sqrt{\rho_2}\sqrt{\rho_1}$, and the penultimate step is the Cauchy-Schwartz inequality. Hence, the equality holds if and only if $U(U_1U_2^\dagger) = I$. Note that in this case, also the first equality holds, and we have $\mathrm{Re}\langle w_1, w_2\rangle = \langle w_1, w_2\rangle \in \mathbb{R}^+$, which provides yet another interpretation of the Uhlmann parallel transport condition as a generalization of the Berry pure-state connection: the phase, given by $\Phi_U = \arg\langle w_1, w_2\rangle$, is trivial, i.e., zero.

Given a curve of density matrices $\gamma: [0, 1] \ni t \mapsto \rho(t)$ and the initial amplitude $w(0)$ of $\rho(0)$, the Uhlmann parallel transport gives a unique curve of amplitudes $w(t)$ with the property that $w(t)$ is parallel to $w(t + \delta t)$ for an infinitesimal δt (the horizontal lift of γ). The length of this curve of amplitudes, according to the metric induced by the Frobenius inner product, is equal to the length, according to the Bures metric (which is the infinitesimal version of the Bures distance $D_B(\rho_1, \rho_2)^2 = 2[1 - F(\rho_1, \rho_2)]$), of the corresponding curve γ of the density matrices. This shows the relation between the Uhlmann connection and the fidelity (for details, see, for example, Refs. [11,41]).

We see that the "Uhlmann factor" U, given by the polar decomposition $\sqrt{\rho(t + \delta t)}\sqrt{\rho(t)} = |\sqrt{\rho(t + \delta t)}\sqrt{\rho(t)}|U$, characterizes the Uhlmann parallel transport. For two close points t and $t + \delta t$, if the two states $\rho(t)$ and $\rho(t + \delta t)$ belong to the same phase, one expects them to almost commute, resulting in the Uhlmann factor being approximately equal to the identity $\sqrt{\rho(t + \delta t)}\sqrt{\rho(t)} \approx |\sqrt{\rho(t + \delta t)}\sqrt{\rho(t)}|$. On the other hand, if the two states belong to two different phases, one expects them to be drastically different (confirmed by the fidelity approach), both in terms of their eigenvalues and/or eigenvectors, potentially leading to nontrivial $U \neq I$ (see the previous study on the Uhlmann factor and the finite-temperature PTs for the case of the BCS superconductivity [16]). To quantify the difference between the Uhlmann factor and the identity, and thus the nontriviality of the Uhlmann connection, we consider the following quantity:

$$\begin{aligned}\Delta(\rho(t), \rho(t + \delta t)) &\coloneqq F(\rho(t), \rho(t + \delta t)) \\ &\quad - \mathrm{Tr}\left[\sqrt{\rho(t + \delta t)}\sqrt{\rho(t)}\right]. \quad (2)\end{aligned}$$

Note that $\Delta = \mathrm{Tr}[|\sqrt{\rho(t + \delta t)}\sqrt{\rho(t)}|(I - U)]$. When the two states are from the same phase we have $\rho(t) \approx \rho(t + \delta t)$, and thus $\Delta \approx 0$. Otherwise, if the two states belong to different phases, and the Uhlmann factor is nontrivial, we have $\Delta \neq 0$. Thus, sudden departure of Δ from zero (for $\delta t \ll 1$) signals the points of PTs. Since both the Uhlmann parallel transport and the fidelity give rise to the same metric (the Bures metric), the nonanalyticity of Δ is accompanied by the same behavior of the fidelity. Note that the other way around is not necessarily true: in case the states commute with each other and differ only in their eigenvalues, the Uhlmann connection is trivial, and thus $\Delta = 0$.

In order for the Uhlmann connection and the fidelity to be in tune, they must be taken over the same base space. In previous studies [13], an Uhlmann connection in 1D translationally invariant systems was considered. The base space considered is the momentum space and the density matrices are of the form $\{\rho_k \coloneqq e^{-\beta H(k)}/Z : k \in \mathcal{B}\}$, where $H(k) = E(k)\vec{n}(k) \cdot \vec{\sigma}/2$ and $\mathcal{B}$ is the first Brillouin zone. Since we are in one dimension, there exists no curvature and hence the holonomy along the momentum space cycle becomes a topological invariant (depends only on the homotopy class of the path). It was found that the Uhlmann geometric phase $\Phi_U(\gamma_c)$ along the closed curve given by $\gamma_c(k) = \rho_k$, changes abruptly from π to 0 after some "critical" temperature T_U. Namely, the Uhlmann phase is given by

$$\Phi_U(\gamma_c) = \arg \mathrm{Tr}\{w(-\pi)^\dagger w(\pi)\} \\ = \arg \mathrm{Tr}\{\rho_\pi U(\gamma_c)\}, \quad (3)$$

where $w(k)$ is the horizontal lift of the loop of density matrices ρ_k, and $U(\gamma_c)$ is the Uhlmann holonomy along the first Brillouin zone. This temperature, though, is not necessarily related to a physical quantity that characterizes a system's phase. It might be the case that the Uhlmann phase is trivial, $\Phi_U(\gamma_c) = 0$, while the corresponding holonomy is not, $U(\gamma_c) \neq I$. For the systems studied in Ref. [13], the Uhlmann holonomy is a smooth function of the temperature and is given, in the basis in which the chiral symmetry operator is diagonal, by

$$U(\gamma_c) = \exp\left\{-\frac{i}{2}\int_{-\pi}^{\pi}\left[1 - \mathrm{sech}\left(\frac{E(k)}{2T}\right)\right]\frac{\partial\varphi}{\partial k}dk\sigma_z\right\}, \quad (4)$$

where $\varphi(k)$ is the polar angle coordinate of the vector $\vec{n}(k)$ lying on the equator of the Bloch sphere. Note that $\lim_{T\to 0}U(\gamma_c) = e^{-i\nu\pi\sigma_z}$, with the Berry phase being $\Phi_B = \lim_{T\to 0}\Phi_U = \nu\pi$, and ν the winding number. While in this case the Uhlmann phase suffers from an abrupt change (steplike behavior), the Uhlmann holonomy is smooth and there is no PT-like behavior.

In the paradigmatic case of the quantum Hall effect, at $T = 0$, the Hall conductivity is quantized in multiples of the first Chern number of a vector bundle in momentum space through several methods. For example, one can use linear response theory or integrate the fermions to obtain the effective action of an external U(1) gauge field. The topology of the bands appears, thus, in the response of the system to an external field. It is unclear, though, that the former mathematical object, the Uhlmann geometric phase along the cycle of the 1D momentum space, has an interpretation in terms of the response of the system. In order to measure this Uhlmann geometric phase, one would have to be able to change the quasimomentum of a state in an adiabatic way. In realistic setups, the states at finite temperatures are statistical mixtures over all momenta, such as the thermal states considered, and realizing closed curves of states ρ_k with precise momenta changing in an adiabatic way seems a tricky task. The fidelity computed in our Letter though, refers to the change of the system's *overall* state, with respect to its parameters (controlled in the laboratory much like an external gauge field), and is related to an, *a priori*, physically relevant geometric quantity, the Uhlmann factor U. The quantity $\Delta = \mathrm{Tr}[|\sqrt{\rho(t+\delta t)}\sqrt{\rho(t)}|(I-U)]$ contains information concerning the Uhlmann factor, since $U = U(t+\delta t)U^\dagger(t)$, where $U(t) = T\exp\{-\int_0^t \mathcal{A}(d\rho/ds)ds\}$ is the parallel transport operator and $\mathcal{A}$ is the Uhlmann connection differential 1-form (for details, see Ref. [42]).

Results.—In our analysis we probe the fidelity and Δ with respect to the parameters of the Hamiltonian describing the system and the temperature, independently. We perform this analysis for paradigmatic models of TIs (SSH and Creutz ladder) and TSCs (Kitaev Chain) in one dimension. We analytically calculate the expressions for the fidelity and Δ, for thermal states $\rho = e^{-\beta H}/Z$, where β is the inverse temperature (see the Supplemental Material, SM1 [43] for the details of the derivation). We use natural units: $\hbar = k_B = 1$.

Here we focus on the Creutz ladder model, while the results for SSH and the Kitaev chain are presented in the Supplemental Material, SM2 [43], since they are qualitatively the same. The Hamiltonian for the Creutz ladder model [36,37] is given by

$$\mathcal{H} = -\sum_{i\in\mathbb{Z}} K(e^{-i\phi}a_{i+1}^\dagger a_i + e^{i\phi}b_{i+1}^\dagger b_i) \\ + K(b_{i+1}^\dagger a_i + a_{i+1}^\dagger b_i) + Ma_i^\dagger b_i + \mathrm{H.c.}, \quad (5)$$

where a_i, b_i, with $i \in \mathbb{Z}$, are fermion annihilation operators, K and M are hopping amplitudes (horizontal or diagonal and vertical, respectively) and $e^{i\phi}$ is a phase factor associated with a discrete gauge field. We take $2K = 1$, $\phi = \pi/2$. Under these conditions, the system is topologically nontrivial when $M < 1$ and trivial when $M > 1$. Given two close points (M, T) and $(M', T') = (M + \delta M, T + \delta T)$, we compute $F(\rho, \rho')$ and $\Delta(\rho, \rho')$ between the states $\rho = \rho(M, T)$ and $\rho' = \rho(M', T')$. To distinguish the contributions due to the change of the Hamiltonian's parameter and the temperature, we consider the cases $\delta T = 0$ and $\delta M = 0$, respectively; see Fig. 1.

We see that for $T = 0$ both fidelities exhibit a sudden drop in the neighborhood of the gap-closing point $M = 1$, signaling the topological quantum PT. As temperature increases, the drops of both fidelities at the quantum critical point are rapidly smoothened towards the $F = 1$ value. This shows the absence of both finite-temperature parameter-driven, as well as temperature-driven (i.e., thermal) PTs. The plot for Δ, for the case $\delta T = 0$, shows a behavior similar to that of the fidelity, while for $\delta M = 0$ we obtain no information, as Δ is identically equal to zero, due to the triviality of the Uhlmann connection associated with the mutually commuting states (a consequence of the Hamiltonian's independence on the temperature). Δ is sensitive to PTs for which the state change is accompanied by a change of the eigenbasis (in contrast to fidelity, which is sensitive to both changes of eigenvalues and eigenvectors). For TIs and TSCs, this corresponds to parameter-driven transitions only.

We further study a topologically trivial superconducting system, given by the BCS theory, with the effective Hamiltonian

$$\mathcal{H} = \sum_k (\varepsilon_k - \mu)c_k^\dagger c_k - \Delta_k c_k^\dagger c_{-k}^\dagger + \mathrm{H.c.}, \quad (6)$$

where ε_k is the energy spectrum, μ is the chemical potential, Δ_k is the superconducting gap, $c_k \equiv c_{k\uparrow}$ and $c_{-k} \equiv c_{-k\downarrow}$ are operators annihilating, respectively, an electron with

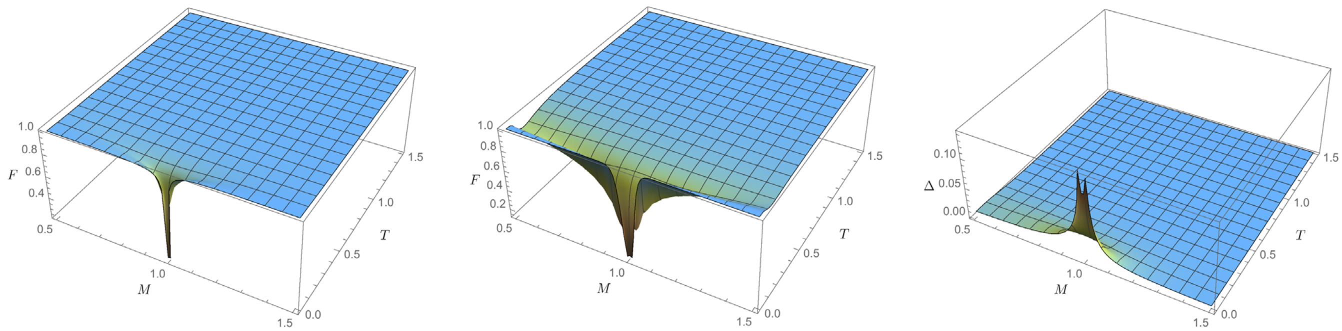

FIG. 1. The fidelity for thermal states ρ, when probing the parameter of the Hamiltonian that drives the topological PT $\delta M = M' - M = 0.01$ (left), and the temperature $\delta T = T' - T = 0.01$ (center), and the Uhlmann connection, when probing the parameter of the Hamiltonian M (right), for the Creutz ladder model (representative of the symmetry class AIII). The plot for Δ when deforming the thermal state along T is omitted since it is equal to zero everywhere.

momentum k and spin-up and an electron with momentum $-k$ and spin-down. The gap parameter is determined in the above mean-field Hamiltonian through a self-consistent mass gap equation and it depends on the original Hamiltonian's coupling associated with the lattice-mediated pairing interaction V, absorbed in Δ_k (for more details, see Ref. [16]). The solution of the equation renders the gap temperature dependent. In Fig. 2, we show the quantitative results for the fidelity and Δ. We observe that both quantities show the existence of thermally driven PTs, as their abrupt change in the point of criticality at $T = 0$, survive and drift, as temperature increases. Unlike TSCs, in this model the temperature does not only appear in the thermal state, but it is also a parameter of the effective Hamiltonian, resulting in the change of the system's eigenbasis and, consequently, nontrivial Uhlmann connection. For a detailed analysis and the explanation of the differences between the two, see the Supplemental Material, SM4 [43].

Finally, we also studied the behavior of the edge states for the TIs and the Majorana modes for the Kitaev chain, on open chains of 500 and 300 sites, respectively. In the case of TIs, we showed that the edge states localized at the boundary between two distinct topological phases, present at zero temperature, are gradually smeared out with the temperature increase, confirming the absence of temperature-driven PTs (see the Supplemental Material, SM3.1 [43] for detailed quantitative results and technical analysis). Our results on the edge states, obtained for systems in thermal equilibrium, agree with those concerning open systems treated within the Lindbladian approach [10] (and, consequently, due to considerable computational hardness, obtained for an open chain of 8 sites). Similarly, we showed that the Majorana modes exhibit an abrupt change at the zero-temperature point of the quantum PT, while the finite-temperature behavior is smooth, confirming the results obtained through the fidelity and the Uhlmann connection analysis (see the Supplemental Material, SM3.2 [43]). In the case of zero-temperature, Majorana modes of the Kitaev model are known to be good candidates for encoding qubit states in stable quantum memories, see Refs. [50,51] and references therein. The presence of robust Majorana modes at low, but finite, temperatures is a significant property which could be used in designing stable quantum memories in realistic setups.

Conclusions and outlook.—We studied the relationship between the fidelity and the Uhlmann connection over the system's *parameter space* (including parameters of the system's Hamiltonian and temperature) and found that their behaviors are consistent whenever the variations of the parameters produce variations in the eigenbasis of the density matrix. By means of this analysis, we showed the absence of temperature-driven PTs in 1D TIs and TSCs. We clarified that the Uhlmann geometric phase considered in *momentum space* is not adequate to infer such PTs, since it is only a part of the information contained in the Uhlmann holonomy. Indeed, this holonomy, as a function of temperature, is smooth [Eq. (4)]; hence, no PT-like phenomenon is expected. Furthermore, we performed the same analysis in the case of BCS superconductivity, where, in contrast to the former

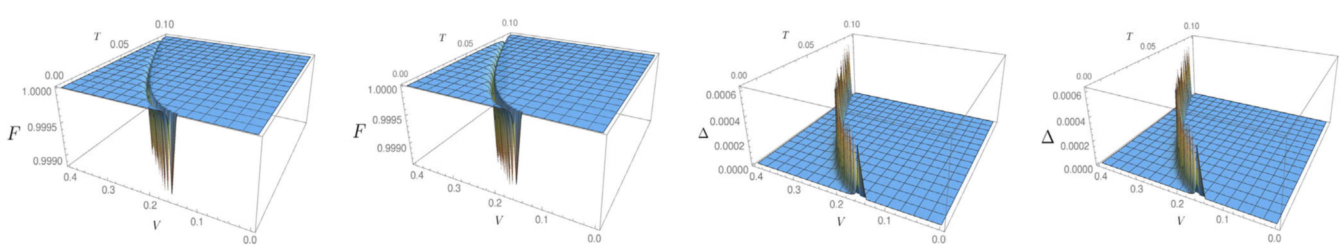

FIG. 2. The fidelity for thermal states ρ when probing the parameter of the Hamiltonian $\delta V = V' - V = 10^{-3}$ (left) and the temperature $\delta T = T' - T = 10^{-3}$ (center left), and the Uhlmann connection (center right and right, respectively), for BCS superconductivity.

systems, thermally driven PTs occur and are captured by both the fidelity and the Uhlmann connection. This shows that, when changing the temperature, the density operator is changing both at the level of its spectrum and its eigenvectors. We analyzed in detail the origin of the differences between the BCS and the Kitaev chain and suggested that in realistic scenarios the gap of topological superconductors could also, generically, be temperature dependent.

Finally, we would like to point out possible future lines of research. The study of Majorana modes at finite temperature suggests that they can be used in achieving realistic quantum memories. This provides a relevant path for future research. Another related subject is to perform the same analysis using an open system approach where the system interacts with a bath and eventually thermalizes. There the parameter space would also include the parameters associated with the system-bath interaction.

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