Dynamical Topological Order Parameters far from Equilibrium

Jan Carl Budich and Markus Heyl
Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, 6020 Innsbruck, Austria and Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria
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Equilibrium phase transitions have a non-equilibrium analog in quantum real-time evolution – coined dynamical quantum phase transitions (DQPTs) – which is driven by progressing time instead of conventional control parameters such as temperature. While the occurrence of DQPTs has recently been reported in various systems, the characterization of the dynamical phases separated by a DQPT in terms of order parameters has remained elusive so far. Here, studying quantum quenches in two-banded Bogoliubov de Gennes models, we identify for the first time a dynamical order parameter that physically distinguishes the involved dynamical phases. More specifically, this novel topological quantum number is a momentum space winding number of the Pancharatnam geometric phase which changes its discrete value only at a DQPT.

The theory of phase transitions is of fundamental importance for our understanding of the variety of phases of matter that occur in nature. Conventional phase transitions in thermal equilibrium are characterized by non-analyticities in thermodynamic potentials such as, e.g., the free energy, as well as in observables and susceptibilities \[1\, 2\]. Usually, the phases separated by such transitions are qualitatively distinguished by an order parameter. More recently, a dynamical counterpart to equilibrium phase transitions, coined dynamical quantum phase transitions (DQPTs), has been discovered in the coherent time evolution of a pure quantum state \[|\psi\rangle\] \[3\], generated by a Hamiltonian \[H\]. These DQPTs appear as a non-analytic behavior at critical times of the Loschmidt amplitude

\[
\mathcal{G}(t) = \langle \psi | \psi(t) \rangle = \langle \psi | e^{-iHt} | \psi \rangle. \tag{1}
\]

In the meantime, DQPTs have been identified in a variety of different systems \[3\, 14\]. Although Loschmidt amplitudes bear a formal similarity to equilibrium partition functions \[3\], this analogy between DQPTs and equilibrium phase transitions does not directly extend to non-analytic behavior in natural observables. In particular, the definition of dynamical order parameters that physically distinguish the dynamical phases separated in time by a DQPT has remained a fundamental open question. Below, we identify for the first time a dynamical order parameter for DQPTs occurring after a quantum quench in two-banded Bogoliubov de Gennes models such as the Kitaev chain \[15\].

DQPTs occur when the time-evolved state vector \[|\psi(t)\rangle\] becomes orthogonal to the initial state \[|\psi\rangle\]. This can be formally understood from the concept of partition function zeros \[1\, 16\, 17\], which occur as so called Fisher zeros in the context of Loschmidt amplitudes \[3\]. This direct relation between DQPTs and wave function orthogonalities guides our intuition towards looking for an observable quantity that is smoothly defined for non-orthogonal state vectors and thus only allowed to behave discontinuously at critical times. The Pancharatnam geometrical phase (PGP) \[18\, 19\] is precisely such a quantity. It was originally introduced \[18\] to define a relative phase for light beams with non-orthogonal polarization and has later been generalized to extend the notion of Berry’s geometric phase \[20\, 21\] to general time evolution with non-orthogonal initial and final states, in particular allowing for non-adiabatic \[22\] and non-cyclic \[19\] dynamics. The geometric background of this construction is that a non-cyclic evolution can be augmented to a cyclic path in a unique way only if the two end states are non-orthogonal, namely by going back from the final to the initial state along a geodesic in projective Hilbert space.

![FIG. 1. (color online) Left panel: Color plot of the Pancharatnam geometric phase \(\phi_{PG}(t)\), Eq. (8), for chemical-potential quenches \(\mu = 0 \rightarrow \mu = 3\) in the Kitaev chain as a function of lattice momentum and time. Time is measured in units of the critical time \(t_c\) where the first dynamical quantum phase transition (DQPT) occurs. The critical momentum \(k_c\) at which non-analyticities occur is marked with a black dotted line. Right panel: Rate function \(g(t) = -N^{-1} \text{Re} \log|\mathcal{G}(t)|^2\) of the Loschmidt echo \(\mathcal{L}(t) = |\mathcal{G}(t)|^2\), see Eq. (1), and the dynamical topological order parameter \(\nu_D(t)\), see Eq. (9), as a function of time. The real-time non-analyticities in \(g(t)\), occurring at odd multiples of \(t_c\) (red dashed lines), define the DQPTs. \(\nu_D(t)\) is constant in between two DQPTs but changes its value at the DQPTs thus serving as a dynamical order parameter.]
Below, we define a momentum-space winding number in terms of the PGP which will serve as a dynamical topological order parameter (DTOP) in two-banded Bogoliubov de Gennes models undergoing a quantum quench, i.e., a sudden change in the band structure parameters. The integer-valued DTOP can only change its value at DQPTs and, moreover, allows us to dynamically resolve how the topology of the underlying Hamiltonian has changed during the quench. Our construction relies on the presence of a so-called particle hole symmetry (PHS), i.e., a spectral constraint imposed by an antiunitary operator $C$, $C^2 = 1$ which anti-commutes with the system Hamiltonian. In Bogoliubov de Gennes models, such a constraint is naturally imposed by the fermionic algebra to the Nambu spinor representation of the Hamiltonian [23]. We illustrate our construction by studying quenches in representative models, one of which is the Kitaev chain [15].

**Underlying Hamiltonian** – The dynamical properties we are concerned with here are generated by gapped free fermionic two-banded Bogoliubov de Gennes models in 1D without requiring further symmetries, i.e., in symmetry class D [23]. We denote the Nambu pseudo-spin by $\tau$ and choose the convention $C = \tau_1 K$ for the PHS operation, where $K$ denotes the complex conjugation. We measure lengths in units of the lattice constant so that the first Brillouin zone is the circle resulting from the interval $[-\pi, \pi]$ by identification of its end points. The Bloch Hamiltonian is then of the form

$$H(k) = \vec{d}(k) \cdot \vec{\tau} = \sum_{j=1}^{3} d^j(k) \tau_j$$

and satisfies the spectral PHS constraint

$$\tau_1 H(k) \tau_1 = -H^*(-k).$$

As a consequence of Eq. (3), $d^i(k)$ and $d^j(k)$ must be odd functions of the lattice momentum $k$, while $d^3(k)$ must be even. Eq. (3) is local in momentum at the two real lattice momenta $k_\pi = 0, \pi$ which satisfy $k = -k \ (\text{mod} 2\pi)$ and where both $d^1$ and $d^2$ need to vanish such that

$$H(k_\pi) = d^3(k_\pi) \tau_3, \quad k_\pi \in \{0, \pi\}.$$  (4)

With the unit vector $\vec{d}(k) = \vec{d}(k)/|\vec{d}(k)|$, the simple geometrical interpretation of Eq. (4) is that $\vec{d}$ is pinned to the poles of the Bloch sphere at the real momenta which plays a crucial role in the following. There are two topologically inequivalent classes of such Hamiltonians [14], in our notation simply distinguished by the sign of $d^3(0)d^3(\pi)$ which becomes negative for the non-trivial topological phase.

**Quench dynamics and DQPTs** – In the following, we study nonequilibrium quantum real-time evolution and DQPTs induced by a quantum quench. The system is prepared in the ground state $|\psi\rangle$ of an initial Hamiltonian $H_i(k) = \vec{d}_i(k) \cdot \vec{\tau}$. At time $t = 0$, a parameter will be switched suddenly within the set of models in Eq. (2) resulting in a sudden change $\vec{d}_i(k) \rightarrow \vec{d}_f(k)$. We assume that the system initially occupies the lower Bloch band of $H_i$. The associated lower Bloch states are denoted by $|u_k^-\rangle$ such that the initial state $|\psi\rangle$ is a Slater determinant of all lower band Bloch states. Since lattice translation invariance is maintained at all times, the dynamics of the system can be considered separately for every lattice momentum $k$. Explicitly, we get

$$|\psi_k(t)\rangle = e^{i\epsilon_k t} g_k |u_k^-\rangle + e^{-i\epsilon_k t} e_k |u_k^+\rangle,$$  (5)

where $\pm \epsilon_k = \pm |\vec{d}_f(k)|$ denotes the energy eigenvalues of $H_f(k)$, $|u_k^\pm\rangle$ its Bloch states, and $g_k = \langle u_k^- | u_k^\pm \rangle$, $e_k = \langle u_k^+ | u_k^- \rangle$ with $|g_k|^2 = \frac{1}{2} (1 + \langle \vec{d}_i(k) \cdot \vec{d}_f(k) \rangle)$, $|e_k|^2 = \frac{1}{2} (1 - \langle \vec{d}_i(k) \cdot \vec{d}_f(k) \rangle)$ are expansion coefficients of the initial lower Bloch state in the new Bloch states after the quench. For the geometric interpretation of our later results, it is helpful to consider the vector $\vec{d}_i(k)$ as a reference direction, say pointing to the south pole of a Bloch sphere defined at every momentum, and to consider the direction of $\vec{d}_f(k)$ relative to this reference. We refer to this construction as the relative Bloch sphere in the following.

Recently, DQPTs in topological systems satisfying Eq. (2) as well as in related spin chains have been identified [3, 10, 14]. DQPTs are caused by Fisher zeros [3] where for a momentum $k_c$ the overlap $\langle u_k^- | \psi_k(t_c) \rangle = 0$ vanishes at a time $t_c$. Here, this can only happen if

$$|g_{k_c}|^2 = |e_{k_c}|^2 = t_{c,n} = \frac{(2n - 1)\pi}{2 e_{k_c}}, \quad n \in \mathbb{N}.$$  (6)

Fisher zeros and DQPTs hence occur at momenta where the initial lower Bloch state is an equal weight superposition of the final Bloch states, i.e. at $\vec{d}_i(k_c) \cdot \vec{d}_f(k_c) = 0$ marking the equator of the relative Bloch sphere, whereas the critical time is determined by the spectrum $\epsilon_k^c$ of the final Hamiltonian.

**Pancharatnam geometric phase** – In order to define the PGP at lattice momentum $k$, let us decompose the Loschmidt amplitude $G(t) = \prod_{k>0} G_k(t)$ with

$$G_k(t) = \langle u_k^- | \psi_k(t) \rangle = r_k(t)e^{i\phi_k(t)}.$$  (7)

and $r_k(t), \phi_k(t)$ its polar coordinates. The phase $\phi_k(t)$ contains a purely geometric and gauge-invariant component

$$\phi^G_k(t) = \phi_k(t) - \phi^dyn_k(t),$$  (8)

obtained by subtracting the dynamical phase $\phi^{dyn}_k(t) = -\int_0^t ds \langle \psi_k(s) | H_f | \psi_k(s) \rangle = \epsilon_k t (|g_k|^2 - |e_k|^2)$.
\( \phi^G_k \) is the above mentioned PGP \[19\] that will be the central building block for the DTOP discovered in this work. We stress that this definition of the PGP becomes singular at Fisher zeros as the total phase \( \phi_k(t) \) in Eq. \[7\] is ill-defined at critical times.

**Definition of the DTOP** – Eq. \[1\] implies that either \( |\epsilon_k|^2 = 0 \) and \( |g_k|^2 = 1 \) or vice versa at the real momenta \( k_R = 0, \pi \). From Eq. \[3\], we directly conclude that \( \phi_k(t) = \epsilon_k(t)^{\text{dyn}} \), i.e., that the PGP is pinned to zero at these special momenta. Thus, as far as the PGP is concerned, the interval \([0, \pi]\) between the real momenta can be endowed with the topology of the unit circle \( S^1 \) by identifying its end points. We refer to this periodic structure as the effective Brillouin zone (EBZ). We are now ready to define a DTOP in terms of the PGP as

\[
\nu_D(t) = \frac{1}{2\pi} \int_0^\pi \frac{\partial \phi^G_k(t)}{\partial k} \, dt. \tag{9}
\]

\( \nu_D(t) \) is the integer-quantized winding number of the PGP over the EBZ and is smoothly defined as a function of time in the absence of Fisher zeros. More formally, \( \nu_D(t) \) is a topological invariant distinguishing homotopically inequivalent mappings \( \text{EBZ} \rightarrow U(1) \), \( k \mapsto e^{i\phi^G_k(t)} \) from the unit circle \( S^1 \) to itself. The definition of \( \nu_D(t) \) in Eq. \[9\] and its subsequent further interpretation as a DTOP are the main results of our present work.

Since DQPTs can only occur at points in time where Fisher zeros are present, \( \nu_D(t) \) must be constant in time intervals between DQPTs as it cannot smoothly change its integer value. But does \( \nu_D \) change its value at every DQPT? We answer this question in the affirmative implying that \( \nu_D(t) \) serves as an order parameter for the studied DQPTs. We find that, quite remarkably, the change in the DTOP \( \Delta \nu_D(t_c) \) in the vicinity of a critical time \( t_c \) can be directly related to the sign of the slope \( s_{k_c} = (\partial_k |\epsilon_k|^2)_{k_c} \) at the critical momentum as

\[
\Delta \nu_D(t_c) = \lim_{\tau \to 0} \left[ \nu_D(t_c + \tau) - \nu_D(t_c - \tau) \right] = \text{sgn}(s_{k_c}) \tag{10}
\]

which loosely resembles an index theorem. This result affords an intuitive geometric interpretation: As pointed out before, critical momenta are located on the equator of the relative Bloch sphere. \( \Delta \nu_D(t_c) \) is then directly related to whether \( \hat{d}_f(k) \) traverses the equator of the relative Bloch sphere from the northern to the southern hemisphere (\( \text{sgn} \left( s_{k_c} \right) = -1 \)) or from the southern to the northern hemisphere (\( \text{sgn} \left( s_{k_c} \right) = 1 \)) at the critical momentum.

To establish Eq. \[10\], we first identify a fundamental dynamical symmetry of \( G_k(t) \) (see Eq. \[7\]) at critical momenta \( k_c \): From Eqs. \[5\] and \[6\], we conclude that \( G_k(t_c) \in \mathbb{R} \). Furthermore, the dynamical phase is zero due to \( |g_{k_c}|^2 = |\epsilon_{k_c}|^2 \) such that \( e^{i\phi^G_{k_c}(t)} = \text{sgn} \left( \cos(\epsilon^f_{k_c} t) \right) \), i.e., the PGP is pinned to the real values 0, \( \pi \) at the critical momenta at all times. When passing through critical times, marked by \( \cos(\epsilon^f_{k_c} t_c) = 0 \), the sign of \( \cos(\epsilon^f_{k_c} t) \) changes and the PGP jumps by \( \pi \). Expanding \( \partial_k \phi^G_{k_c}(t) \) around \( k_c \) and \( t_c \) to leading order, it is straightforward to prove Eq. \[10\].

**Benchmarks** – We further investigate and illustrate the DTOP \( \nu_D(t) \) with two benchmark examples. First, we study a model that was originally introduced by Kitaev \[15\] as a toy model for a proximity induced \( p \)-wave superconductor. The model Hamiltonian is of the form \[2\] with \( d^1(k) = 0, \ d^2(k) = \sin(k), \ d^3(k) = \mu - \cos(k) \), where physically the \( \cos(k) \) term represents the kinetic energy and the \( \sin(k) \) term represents the \( p \)-wave pairing. Here, we would like to perform a quench in the chemical potential \( \mu \) which changes from \( \mu = 0 \) in the initial Hamiltonian \( H_i \) to \( \mu = 3 \) in the final Hamiltonian \( H_f \). At the real momentum \( k = 0 \) the \( d^0 \) component changes sign over the quench while at \( k = \pi \) it does not, meaning that the topological phase of the Hamiltonian \[15\] changes during the quench. Hence, \( |\epsilon_0|^2 = 1 \) while \( |\epsilon_\pi|^2 = 0 \). Due to continuity, there must be a critical momentum \( k_c \) in the interior of the EBZ where \( |\epsilon_{k_c}|^2 = |g_{k_c}|^2 = \frac{1}{2} \) in agreement with Ref. \[14\]. According to Eq. \[6\] and \[10\], this implies that DQPTs will occur at times \( t_{c,n} = (2n - 1)\pi/(2|\epsilon_{k_c}|) = (2n - 1)t_c, \ n \in \mathbb{N} \). More specifically we find, \( k_c = \arccos(1/3), \ t_c = \pi/(4\sqrt{2}) \) and \( s_{k_c} = -1 \), i.e., \( \hat{d}_f(k) \) crosses the equator of the relative Bloch sphere in southern direction, corresponding to a change \( \Delta(t_{c,n}) = -1 \) in the DTOP (see Eq. \[10\] at the critical times \( t_{c,n} = (2n - 1)t_c \). In Fig. \[1\] we show a color-plot of the PGP as a function of \( k \) and \( t \) from which the critical times and the associated changes in the phase winding number \( \nu_D \) representing our DTOP become visually clear (left panel). Moreover,
Fig. 1 displays the time dependence of both the DTOP $\nu_D(t)$ and the rate function $g(t) = -N^{-1}\log(|\mathcal{G}(t)|^2) = -\pi^{-1}\Re \left( \log \int_0^\pi dk \left[ |g_k|^2 + e^{-2i\nu_D^t|e_k|^2} \right] \right)$ which plays the role of a thermodynamic potential here and whose points of nonanalytic behavior define the DQPTs \[3\] (right panel). The DTOP indeed changes its value at every DQPT and uniquely characterizes the dynamical phase in between two DQPTs.

As a second benchmark, we consider a quench from $d_i(k) = (0, 0, 1)$ to $d_f(k) = (0, \sin(k), 1 + \cos(2k) + \lambda\cos(k))$. This model is similar to the Kitaev chain studied before, but also includes a next-to-nearest neighbor hopping. For $0 < \lambda < 2$, this quench does not change the topological phase of the Hamiltonian since $d_i(k_R) = d_f(k_R)$. Still, from Eq. \[6\] we find two critical momenta $k_c^{(1)} = \pi/2$, $k_c^{(2)} = \arccos(-\lambda/2)$. At $k_c^{(1)}$, $d_f(k)$ enters the northern hemisphere of the relative Bloch sphere and returns to the southern hemisphere at $k_c^{(2)}$, i.e., $d_i(k) \cdot d_f(k) < 0$ for $k_c^{(1)} < k < k_c^{(2)}$. As a consequence, $\text{sgn}(s_{k_c^{(1)}}^i) = -\text{sgn}(s_{k_c^{(2)}}^i) = 1$ and, from Eq. \[10\], we see that the change in the DTOP is opposite at the two critical momenta. In Fig. 2 we again show a color plot of the PGP for this quench (left panel) as well as the time dependence of the rate function $g(t)$ and the DTOP $\nu_D(t)$ (right panel). The DTOP changes at every DQPT, however, due to the competing $\Delta(t_{c,n}^{(i)}) = (-1)^{i+1}$, $i = 1, 2$, its behavior is not monotonous as opposed to the first quench example.

Concluding discussion – The DTOP $\nu_D$ (see Eq. \[9\]) discovered in this work qualitatively distinguishes dynamical phases that are separated in time by a DTOP. We would like to emphasize that the DTOP as a truly dynamical quantity is fundamentally different from the conventional topological invariants that classify ground states of gapped Hamiltonians \[24-26\]. In particular, if we calculate for the time dependent many-body state $|\psi(t)\rangle$ the conventional topological invariant at every point in time, it turns out to be a constant of motion in our present non-equilibrium setting \[9, 27, 28\]. However, there still is an interesting interplay between conventional equilibrium invariants and the occurrence of DQPTs here. In this context, it has been recently shown \[14\] that topologically inequivalent Hamiltonian ground states before and after the quench require the presence of DQPTs, in agreement with the situation in our first benchmark example. However, DQPTs can also happen if the initial and the final Hamiltonian are topologically equivalent as in our second benchmark example. Quite remarkably, the structure of the DTOP is capable of resolving these different scenarios. From Eq. \[10\], we see that the DTOP behaves qualitatively different in these two cases (see also comparison of right panels of Fig. 1 and Fig. 2). If the Hamiltonian topology changes over the quench, there is an odd number of critical momenta thus giving rise to a change of the DTOP after one DQPT associated with each of the critical momenta. In contrast, if the initial and final Hamiltonians are equivalent, the sum over the changes of $\nu_D$ for all critical momenta is zero.

We emphasize that the construction of the DTOP relies on the two-handed character of the models we consider. For larger unit cells, pertaining in particular to the modelling of disordered systems, the change of the PGP between the real momenta is not necessarily quantized because the spectral PHS constraint in Eq. \[3\] does not enforce Eq. \[4\]. However, in many physical situations considering an effective model with two bands is a physically well justified approximation and the DTOP defined here is hence also expected to emerge in the low energy theory of more complex systems. The generalization of our present construction to higher spatial dimensions is not straightforward and may be an interesting subject of future work.

The dynamical order parameter discovered in this work is of topological nature. A natural question is whether also local dynamical order parameters can exist. Although a general answer is beyond the scope of this work, it is still possible to give some intuition. In particular, a dynamical analog of a diverging correlation length, as it appears at continuous equilibrium phase transitions and which would give rise to a nonanalytic behavior of a local observable, cannot develop dynamically in a finite period of time. This is due to fundamental constraints by causality such as Lieb-Robinson bounds. Hence, we do not expect direct analogs of such phenomena at DQPTs.

We conclude by summarizing some recent experimental progress on the building blocks of a setup where DQPTs and the DTOP discovered in this work could be observed. Models similar to the Kitaev chain \[15\], see our benchmark examples, can be realized both in solid state systems \[29-35\] as well as potentially in the context of cold atoms in optical lattices \[36, 37\]. While inducing nonequilibrium quantum real-time evolution in solid state systems is challenging, with ultracold atoms in optical lattices quantum quenches have already been studied experimentally in various contexts \[38, 39\]. Moreover, in such synthetic systems momentum-resolved phase differences of Bloch wave functions, needed for the DTOP defined in Eq. \[9\], have been measured in terms of Berry phases \[40, 41\]. Paving the way towards the observation of DQPTs, a measurement scheme for Loschmidt echos $\mathcal{L}(t) = |\mathcal{G}(t)|^2$ has been recently introduced \[42, 43\].

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