Dynamical Quantum Phase Transitions in the Kitaev Honeycomb Model

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The notion of a dynamical quantum phase transition (DQPT) was recently introduced in [Heyl et al., Phys. Rev. Lett. 110, 135704 (2013)] as the non-analytic behavior of the Loschmidt echo at critical times in the thermodynamic limit. In this work the quench dynamics in the ground state sector of the two-dimensional Kitaev honeycomb model are studied regarding the occurrence of DQPTs. For general two-dimensional systems of BCS-type it is demonstrated how the zeros of the Loschmidt echo coalesce to areas in the thermodynamic limit, implying that DQPTs occur as discontinuities in the second derivative. In the Kitaev honeycomb model DQPTs appear after quenches across a phase boundary or within the massless phase. In the 1d limit of the Kitaev honeycomb model it becomes clear that the discontinuity in the higher derivative is intimately related to the higher dimensionality of the non-degenerate model. Moreover, there is a strong connection between the stationary value of the rate function of the Loschmidt echo after long times and the occurrence of DQPTs in this model.

I. INTRODUCTION

Recent advances in experimental techniques allow to realize closed quantum systems with cold atomic gases in optical traps. These setups are precisely controllable and the unitary time evolution of the systems can be resolved such that the dynamics are experimentally accessible under well-known conditions. Motivated by the new experimental possibilities a lot of theoretical research on the non-equilibrium dynamics of quantum systems has been conducted in the past years. In these theoretical investigations a common protocol for driving a system out of equilibrium is called quantum quench. Considering a parametrised Hamiltonian $H(\alpha)$, where the parameter typically corresponds to some external field strength in the experimental setup, the system is initially assumed to be in equilibrium with regard to some value $\alpha_i$ of the parameter. Then, the parameter is suddenly quenched to a different final value $\alpha_f$ driving the system out of equilibrium and inducing a non-trivial time evolution.

Studying the quench dynamics of a quantum many-body system, Heyl et al. pointed out the close formal similarity of the canonical partition function of an equilibrium system, $Z(\beta) = \text{tr} (e^{-\beta H})$, and the return amplitude

$$ G(t) = \langle \psi_i | e^{-iHt} | \psi_i \rangle $$

of a time-evolved state, suggesting the possibility of critical behavior in the time evolution in analogy to equilibrium phase transitions. It is known that in the thermodynamic limit the zeros of a partition function coalesce to lines in the complex temperature plane and the equilibrium phase transition is marked by the intersection of the zero-line with the real temperature axis. Heyl et al. found that in the case of the transverse field Ising model the boundary partition function

$$ Z(z) = \langle \psi_i | e^{-zH} | \psi_i \rangle $$

has zeros in the complex time plane, which accordingly coalesce to lines in the thermodynamic limit. These lines cross the real time axis after quenching the external field across the quantum critical point inducing nonanalyticities in the rate function of the Loschmidt echo

$$ r(t) = - \lim_{N \to \infty} \frac{1}{N} \ln |\langle \psi_i | e^{-iHt} | \psi_i \rangle|^2 $$

at equidistant critical times $t_n^*$. Heyl et al. denote this non-analytic behavior at critical times in the thermodynamic limit as a dynamical quantum phase transition (DQPT). They showed that in experiment the DQPT would be observable by measuring the work distribution function of a double quench; in particular, the Loschmidt echo $\mathcal{L}(t) = |\langle \psi_i | e^{-iHt} | \psi_i \rangle|^2$ is the probability of performing no work.

These findings triggered further work aiming at a better understanding of the phenomenon. By considering an additional integrability-breaking interaction in the transverse field Ising chain it was demonstrated that DQPTs are not a peculiarity specific to integrable models, but are stable against some non-integrable perturbations. Moreover, the signature of DQPTs was found in higher-dimensional systems, namely, in two-dimensional topological insulators and effectively infinite dimensions using DMFT. It was observed in various cases that DQPTs are not necessarily connected to quenching across a quantum critical point, however, there seems to be a strong connection to topological phase transitions. Canovi et al. detected coexisting solutions for so called generalized expectation values in post quench dynamics and, therefore, they introduced the notion of a first order dynamical phase transition. This could be a way to classify dynamical phase transitions. Furthermore, a close connection between the analytic behavior of $r(t)$ in the complex plane and its long time limit is conjectured.

In this work we study quench dynamics in the Kitaev honeycomb model regarding dynamical quantum phase transitions. The model features a rich phase diagram comprising an extended gapless phase, anyonic
excitations, and topological order. Moreover, it is a rare example of a Jordan-Wigner-solvable model in two dimensions.\textsuperscript{15,16} As such it has been studied extensively under various aspects. In this paper we restrict the discussion to the dynamics in the ground state sector.

The dynamics of gapped two-dimensional two-band systems were already studied by Vajna and Dóra with focus on a connection between DQPTs and topological phases.\textsuperscript{17} In the presence of a magnetic field the Kitaev model acquires topological order and becomes a system of the same family, albeit being a spin model. In that case we find the behavior in accordance with their results, namely, DQPTs occur after quenches across the boundary between phases with different Chern number. However, the focus of this work lies on quenching between the topologically trivial phases in the absence of a magnetic field. Similar to their results we find DQPTs as discontinuities in the second derivative, which is inherent to the higher dimensionality of the system, and we elaborate on the relevance of the complex zeros of the dynamical partition function in this context. Moreover, we discuss a remarkable observation regarding the long time behavior of the Loschmidt echo. If no DQPTs occur in the post-quench dynamics, then, although the approached stationary state is always an excited state, the long time limit of the Loschmidt echo is given by the fidelity, i.e., the overlap of the initial state with the ground state of the quenched Hamiltonian. This, however, does not hold if the dynamics exhibit DQPTs.

The rest of this paper is organized as follows: in section II, the way of solving the model using Jordan-Wigner transformation is sketched and the phase diagram is introduced. Furthermore, the expressions for the dynamical free energy is derived. In section III, the zeros of the dynamical partition function in the complex time plane are treated assuming a general BCS-type Hamiltonian, yielding the criteria for the occurrence of DQPTs and the order of the corresponding nonanalyticity. Finally, the zeros of the partition function and the real time evolution are studied explicitly for the Kitaev model in section IV and two interesting limits are taken into account as well as ramping as an alternative protocol and the quenching with an additional magnetic field.

II. THE KITAEV HONEYCOMB MODEL

A. The model

The Kitaev honeycomb model is defined by the Hamiltonian

\[ H(\vec{J}) = - \sum_{\alpha \in \{x,y,z\}} \sum_{\text{-links}} J_{\alpha} \sigma_\alpha^x \sigma_\alpha^y, \]

which describes a spin-1/2 system with the spins located on the vertices (labeled by \( j, k \)) of a honeycomb lattice as depicted in Fig. 1. In this paper we assume the lattice spacing to equal unity. It has been shown\textsuperscript{16} that for the above Hamiltonian one can find a Jordan-Wigner contour, which after identifying a conserved \( Z_2 \) operator and switching to momentum space yields a BCS-type Hamiltonian

\[ H(\vec{J}) = \sum_{\vec{k}} \left[ \frac{\epsilon_{\vec{k}}(\vec{J})}{2} \left( d_\vec{k}^\dagger d_\vec{k} - d_{-\vec{k}}^\dagger d_{-\vec{k}} \right) + \frac{\Delta_{\vec{k}}(\vec{J})}{2} \left( d_\vec{k}^\dagger d_{-\vec{k}} + d_{-\vec{k}}^\dagger d_\vec{k} \right) \right] \]

with

\[ \epsilon_{\vec{k}}(\vec{J}) = 2(J_z + J_x \cos(k_z) + J_y \cos(k_y)), \]

\[ \Delta_{\vec{k}}(\vec{J}) = 2(J_x \sin(k_x) + J_y \sin(k_y)). \]  

This Hamiltonian can be diagonalised by a Bogoliubov transformation

\[ \begin{pmatrix} a_\vec{k}^\dagger \\ a_{-\vec{k}}^\dagger \end{pmatrix} = \begin{pmatrix} u_{\vec{k}}(\vec{J}) & v_{\vec{k}}(\vec{J}) \\ -v_{\vec{k}}(\vec{J})^* & u_{\vec{k}}(\vec{J})^* \end{pmatrix} \begin{pmatrix} d_\vec{k}^\dagger \\ d_{-\vec{k}}^\dagger \end{pmatrix}, \]

where

\[ u_{\vec{k}}(\vec{J}) = \sqrt{\frac{1}{2} \left( 1 + \frac{\epsilon_{\vec{k}}(\vec{J})}{E_{\vec{k}}(\vec{J})} \right)}, \]

\[ v_{\vec{k}}(\vec{J}) = \text{sgn}(\Delta_{\vec{k}}(\vec{J})) \sqrt{\frac{1}{2} \left( 1 - \frac{\epsilon_{\vec{k}}(\vec{J})}{E_{\vec{k}}(\vec{J})} \right)} \]  

(see appendix A for details). Plugging the transformation into eq. (5) yields the diagonal Hamiltonian

\[ H(\vec{J}) = \sum_{\vec{k} \in K} \frac{E_{\vec{k}}(\vec{J})}{2} \left( a_{\vec{k}}^\dagger a_{\vec{k}} - a_{-\vec{k}}^\dagger a_{-\vec{k}} \right) \]

with spectrum

\[ E_{\vec{k}}(\vec{J}) = \sqrt{\epsilon_{\vec{k}}(\vec{J})^2 + \Delta_{\vec{k}}(\vec{J})^2}. \]  

FIG. 1. Lattice of the Kitaev honeycomb model given by eq. (1). Spin-1/2 degrees of freedom are sitting on the vertices of a honeycomb lattice. The nearest neighbor interaction depends on the link type \((x, y, \text{ or } z)\).
one half of the Brillouin-zone, e.g., all $\mathbf{k}$. The gapped phase $B$ is surrounded by three gapped phases $A_x$, where $J_x > J_y + J_z$.

The Hamiltonian splits into a sum over $\mathbf{k}$-sectors, i.e., a sum over $\mathbf{k} \in K$, where $K$ is a subset of the Brillouin-zone such that $\forall k \in K, -k \notin K$. A possible choice is one half of the Brillouin-zone, e.g., all $\mathbf{k}$ with $k_x > 0$.

The spectrum has roots at

$$
k_x = \pm \arccos \left( \frac{J_y^2 - J_z^2}{2J_xJ_z} \right),
$$

$$
k_y = \mp \arccos \left( \frac{J_x^2 - J_z^2}{2J_yJ_z} \right)
$$

if $|J_\alpha| < |J_\beta| + |J_\gamma|$, where $(\alpha, \beta, \gamma)$ is any permutation of $(x, y, z)$. We will in the following only consider non-negative $J_\alpha$ on the $J_x + J_y + J_z = 1$ plane. In this section the above result on the gappedness of the spectrum corresponds to a phase diagram as depicted in Fig. 2.

The gapless phase $B$ at the center of the diagram is surrounded by three distinct gapped phases $A_x$, $A_y$ and $A_z$, where $J_x > J_y + J_z$, $J_y > J_z + J_x$ or $J_z > J_y + J_x$, respectively.

In the presence of a magnetic field $\mathbf{h}$ the spin Hamiltonian \( H \) becomes

$$H(\mathbf{J}, \mathbf{h}) = -\sum_{\alpha \in \{x, y, z\}} \left( \sum_{\alpha-\text{links}} J_\alpha a^\dagger_\alpha a^\alpha + \sum_j h_\alpha a^\alpha_j \right)
$$

and the additional term opens a gap also in the $B$-phase. Moreover, the $B$-phase becomes topologically non-trivial with Chern-number $\nu = \pm 1$, whereas the $A_\alpha$ phases remain trivial with $\nu = 0$. At $J_x = J_y = J_z = J$ there exists a diagonal form of the Hamiltonian even with non-zero magnetic field, and the spectrum reads

$$E_{\mathbf{k}}(J, h) = \sqrt{\epsilon_{\mathbf{k}}(J, \kappa)^2 + |\Delta_{\mathbf{k}}(J, \kappa)|^2}
$$

with $\epsilon_{\mathbf{k}}(J, \kappa) = \epsilon_{\mathbf{k}}^B(\mathbf{J}), \mathbf{J} = (J, J, J)^T$ and

$$\Delta_{\mathbf{k}}(J, \kappa) = \Delta_{\mathbf{k}}^B(\mathbf{J}) + 4i\kappa (\sin(k_x) - \sin(k_y) + \sin(k_y - k_x))
$$

where $\kappa \sim \frac{k_x h_y h_z}{E_G}$. Through a Bogoliubov transformation (see appendix A) this maps to

$$H(J, \kappa) = \sum_{k \in K} \left[ \frac{\tilde{\epsilon}_k(J, \kappa)}{2} \left( d^\dagger_k d_k - d_{-k}^\dagger d_{-k} \right) \right. 
$$

$$+ \frac{\Delta_k(J, \kappa)^*}{2} d^\dagger_{-k} d_{-k} + \frac{\Delta_k(J, \kappa)}{2} d_k d_{-k} \right].
$$

This case will be studied in section IV F. Before, we will stick to the case without magnetic field, i.e., real valued $\epsilon_k$ and $\Delta_k$.

B. Post-quench dynamics

In order to study the dynamics in the Kitaev honeycomb model we will consider situations where the system is initially, at $t < 0$, prepared in the ground state of $H(\mathbf{J}_0)$, i.e., $H(\mathbf{J}_0)|\psi_i\rangle = E_{GS}|\psi_i\rangle$. In terms of the free fermion degrees of freedom the initial state is the vacuum: $a^\dagger_{\mathbf{k}}|\psi_i\rangle = a^\dagger_{\mathbf{k}}|0; \mathbf{J}_0\rangle = 0$. At $t = 0$ the parameter is quenched to its final value $\mathbf{J}_1$, such that for $t > 0$ the time-evolved state is $|\psi(t)\rangle = e^{-iH(\mathbf{J}_1)t}|\psi_i\rangle$. Making use of the Bogoliubov transformation the initial state can be expressed in terms of the final free fermions, which diagonalize $H(\mathbf{J}_1)$:

$$|\psi_i\rangle = N^{-1} \prod_{k \in K} \left( 1 + B_{\mathbf{k}}(\mathbf{J}_0, \mathbf{J}_1)a^\dagger_{\mathbf{k}} a_{-\mathbf{k}}^\dagger \right) |0; \mathbf{J}_1\rangle
$$

Here,

$$B_{\mathbf{k}}(\mathbf{J}_0, \mathbf{J}_1) \equiv \frac{V_{\mathbf{k}}(\mathbf{J}_0, \mathbf{J}_1)}{U_{\mathbf{k}}(\mathbf{J}_0, \mathbf{J}_1)} = \frac{u_{\mathbf{k}}(\mathbf{J}_0)v_{\mathbf{k}}(\mathbf{J}_1) - u_{\mathbf{k}}(\mathbf{J}_1)v_{\mathbf{k}}(\mathbf{J}_0)}{u_{\mathbf{k}}(\mathbf{J}_1)v_{\mathbf{k}}(\mathbf{J}_0) + v_{\mathbf{k}}(\mathbf{J}_1)v_{\mathbf{k}}(\mathbf{J}_0)}
$$

and the normalization constant

$$N^2 \equiv \prod_{k \in K} \left( 1 + B_{\mathbf{k}}(\mathbf{J}_0, \mathbf{J}_1)^2 \right)
$$

were introduced. A more detailed derivation is given in appendix A.

For the sake of brevity and lucidity we will in the following refrain from dragging along the dependencies on $\mathbf{J}_0$ and $\mathbf{J}_1$ explicitly, i.e., identify $B_{\mathbf{k}} \equiv B_{\mathbf{k}}(\mathbf{J}_0, \mathbf{J}_1)$ and $a_{\mathbf{k}} \equiv a_{\mathbf{k}}^F$.

Using (16) to compute the dynamical partition function we obtain

$$Z(z) = \langle \psi_i | e^{-zH} | \psi_i \rangle
$$

$$= \prod_{k \in K} \frac{1 + B_{\mathbf{k}}^2 z^2}{1 + B_{\mathbf{k}}^2 z^2}. \quad (19)$$
The dynamical partition function has large deviation form $Z(z) \sim e^{-N f(z)}$, where $N$ is the system size. Thus, in the thermodynamic limit only the rate function, or dynamical free energy density,

$$f(z) = -\lim_{N \to \infty} \frac{1}{N} \ln(Z(z))$$

is well defined.

III. ZEROS OF THE PARTITION FUNCTION AND CRITICAL TIMES

A. General aspects

From the study of equilibrium phase transitions it is known that a very insightful approach is to consider the zeros of the partition function in the complex temperature or complex magnetization plane, respectively.\(^\text{14,19,20}\) In the thermodynamic limit the zeros of the partition function coalesce to lines or areas in the complex plane, which mark the critical points when approaching the real temperature (magnetization) axis. Analogous reasoning has proven useful in the study of dynamical quantum phase transitions.\(^\text{17}\)

In particular, an interesting analogy to electrodynamics allows to characterize the dynamical phase transition through the density of zeros of the dynamical partition function in the complex time plane. The starting point is the observation that the dynamical partition function\(^\text{19}\) is an entire function of $z$ and can be such, according to the Weierstrass factorization theorem, be written as

$$Z(z) = e^{h(z)} \prod_{j \in J} \left(1 - \frac{z}{z_j}\right),$$

where $J$ is some discrete index set, $z_j \in \mathbb{C}$ are the zeros, and $h(z)$ is an entire function. With this, the dynamical free energy density reads

$$f(z) = -\lim_{N \to \infty} \frac{1}{N} \left[h(z) + \sum_{j \in J} \ln \left(1 - \frac{z}{z_j}\right)\right].$$

From this expression it becomes clear, that any nonanalytic behavior of the dynamical free energy can only occur at or in the vicinity of the zeros of the dynamical partition function $z_j$. Since we are interested in nonanalyticities, we will in the following ignore the contribution of $h(z)$ and only consider the singular part

$$f^*(z) = -\lim_{N \to \infty} \frac{1}{N} \sum_{j \in J} \ln \left(1 - \frac{z}{z_j}\right).$$

In the thermodynamic limit the sum becomes an integral over some continuous variable $x \in X$, where $X \subseteq \mathbb{R}$ is a region corresponding to the previously used index set $J$, and the zeros become a function of this variable $\tilde{z}(x)$, such that

$$f^*(z) = -\int_X dx \ln \left(1 - \frac{z}{\tilde{z}(x)}\right).$$

A transformation of the integration variable yields

$$f^*(z) = -\int_{z(X)} d\tilde{z} \rho(\tilde{z}) \ln \left(1 - \frac{z}{\tilde{z}}\right),$$

where the Jacobian determinant $\rho(\tilde{z})$ can be interpreted as the density of zeros in the complex plane.\(^\text{21}\) Moreover, setting $\rho(z) \equiv 0$ for $z \notin z(X)$ allows to extend the integration domain to the full complex plane. We will now discuss the real part

$$\phi(z) = \text{Re} \left[f^*(z)\right] = -\int_{\mathbb{C}} d\tilde{z} \rho(\tilde{z}) \ln \left|1 - \frac{z}{\tilde{z}}\right|.$$

We will later see that the Loschmidt echo on the real time axis is directly given by $\phi(t)$. For $z = x + iy$ with $x, y \in \mathbb{R}$ in $|z|$ is the Green’s function of the Laplacian $\Delta_{2D} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$, i.e.,

$$\Delta_{2D} \phi(z) = -2\pi \rho(z).$$

In other words, the real part of the dynamical free energy density can be interpreted as the electrostatic potential $\phi(z)$ produced by a charge density $\rho(z)$ in two dimensions and the question of the behavior of the free energy at critical points becomes the question of the behavior of the electrostatic potential at surfaces. If the zeros form lines in the complex plane, this allows to deduce the order of the phase transition directly from the density of zeros at or in the vicinity of the physically relevant $z$.\(^\text{20}\)

Although the zeros can form areas in the complex plane these do not cover the physical axis in the case of equilibrium phase transitions. However, as we will see in the following section, this is possible in the case of dynamical phase transitions. Thus, consider the situation as depicted in Fig. 3. The density of zeros is given by $\rho_1(z)$ and $\rho_2(z)$ in area $I$ and $II$, respectively, and at the

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boundary there is a discontinuous change in the density of zeros. Assume the electric potentials \( \phi_i(z), i = 1, 2 \), solve the Laplace equation \( \Delta \phi(z) = 0 \) with the corresponding density \( \rho_i(z) \). With this a global solution is

\[
\phi(z) = \begin{cases} 
\phi_1(z), & z \in I \\
\phi_2(z), & z \in II 
\end{cases}
\]  
(29)

and we demand continuity of \( \phi(z) \) at the boundary. Let us now focus on the behavior of \( \phi(z) \) at the intersection of the boundary with the real time axis. If we choose the \( x \)-\( y \)-coordinate frame as indicated in Fig. 3, the continuity of \( \phi(z) \) implies that on the boundary

\[
\frac{\partial^2}{\partial y^2} \phi_1(z) - \frac{\partial^2}{\partial y^2} \phi_2(z) = 0 .
\]  
(30)

Since we are interested in the behavior of \( \phi(z) \) in the real time axis, we transform to \( t \)-\( y' \)-coordinates,

\[
t = \frac{x}{\cos \alpha} + \frac{y}{\sin \alpha} ,
\]

\[
y' = y .
\]  
(31)

With the Laplace equation \( \Delta \phi = 0 \) this yields

\[
(\cos \alpha)^{-2} \frac{\partial^2}{\partial t^2} \phi_1(z) + (1 + \sin \alpha^{-1})^2 \frac{\partial^2}{\partial y'^2} \phi_1(z) = -2\pi \rho_1(z) ,
\]  
(32)

and, consequently,

\[
\frac{\partial^2}{\partial t^2} [\phi_1(z) - \phi_2(z)] = -2\pi (\cos \alpha)^2 (\rho_1(z) - \rho_2(z)) .
\]  
(33)

This means, if an area of zeros of the partition function overlaps the real time axis, the second derivative of the free energy is discontinuous.

**B. 2d BCS-type models**

In the Kitaev honeycomb model (and general BCS-type models) the partition function is given by \( \Delta \phi(z) = 0 \), i.e., the zeros in the complex plane are given by

\[
z_n(\bar{k}) = \frac{1}{2E_{k^*}} \left[ \ln \left( B_{k^*}^2 \right) + i\pi(2n+1) \right], \quad n \in \mathbb{Z} .
\]  
(34)

At this point it becomes obvious, that in the thermodynamic limit the double product over \( k_x \) and \( k_y \) in \( \Delta \phi(z) = 0 \) leads to dense areas of zeros in the complex plane, since, generally, \( \partial_{k_x} z_n(\bar{k}) \neq \pm i\partial_{k_y} z_n(\bar{k}) \). These areas of zeros cover parts of the real time axis (\( z = it \)) if \( Re(z_n(\bar{k})) = 0 \), i.e., if

\[
\exists \bar{q} \in K \text{ such that } B_{\bar{q}}^2 = 1 .
\]  
(35)

Dubbing the \( B_{\bar{q}}^2 = 1 \) isoline \( B_1 \subset K \), there are intervals

\[
T_n = \frac{(2n+1)\pi}{2E_{B_1}}, \quad n \in \mathbb{Z}
\]  
(36)

on the real time axis, which are covered by areas of zeros. If the spectrum is gapped, the beginnings \( t_n^b \) and end points \( t_n^e \) of two consecutive intervals \( T_n \) and \( T_{n+1} \) are equidistant with \( t_n^b = t_n^e = \frac{\pi}{2E_{B_1}} \) and \( T_{n+1}^e - T_n^b = \frac{\pi}{2E_{B_1}} \), where \( B_{\bar{q}} \) are momenta minimizing/maximizing \( E_{\bar{q}} \) on the domain given by \( |B_{\bar{q}}| = 1 \). The length of the single intervals \( T_n \) increases linearly with \( n \). However, if the spectrum is gapless, all those intervals extend to infinity.

The condition \( \exists \bar{q} \) allows for a physical interpretation; namely, the occurrence of DQPTs is through a continuity argument related to non-thermal mode occupation. In BCS-type models the mode occupation is given by

\[
\langle n_{\bar{q}} \rangle \equiv \langle a_{\bar{q}}^\dagger a_{\bar{q}} \rangle = \sin^2 \left( \frac{\pi}{2} \arctan \frac{B_{\bar{q}}}{B_{\bar{q}}} \right) .
\]  
(37)

This means for all modes \( \bar{q} \), where the condition \( \exists \bar{q} \) is satisfied, the mode occupation is \( \langle n_{\bar{q}} \rangle = 1/2 \). Let us assume that for any two points in \( K \) there exists a path connecting both points, along which \( \langle n_{\bar{q}} \rangle \) is continuous\(^{32} \) and the existence of modes with \( \langle n_{\bar{q}} \rangle < 1/2 \). Both assumptions should be true for physically relevant models and were found to hold in all cases considered in the Kitaev model. Then, we can set up the following chain of consequences: through the continuity condition, the existence of non-thermally occupied modes \( \bar{k}^+ \) with \( \langle n_{\bar{k}^+} \rangle \geq 1/2 \) implies the existence of modes \( \bar{q}^* \) with \( \langle n_{\bar{q}^*} \rangle = 1/2 \). This in turn is equivalent to the fulfillment of the condition \( \exists \bar{q} \), which implies the occurrence of DQPTs in the time evolution. The mode occupation \( \langle n_{\bar{k}^+} \rangle \geq 1/2 \) is non-thermal in the sense that it cannot be realized by Fermi-Dirac statistics with positive temperature.

An equivalent formulation of condition \( \exists \bar{q} \) is

\[
\exists \bar{q} \in K \text{ such that } \Delta_{\bar{q}}(\alpha_0) \Delta_{\bar{q}}(\alpha_1) + \epsilon_{\bar{q}}(\alpha_0) \epsilon_{\bar{q}}(\alpha_1) = 0 ,
\]  
(38)

where \( \alpha \) is the quench parameter of the BCS-type Hamiltonian, (see appendix\(^{13} \)). From this it becomes clear, that after quenching to a gapless phase there are zeros of the dynamical partition function on the real time axis, since \( E_{\bar{q}}(\alpha) = 0 \) is equivalent to \( \epsilon_{\bar{q}}(\alpha) = \Delta_{\bar{q}}(\alpha) = 0 \). In the mode occupation picture this can be interpreted as follows: when quenching to a gapless phase, excitations cost no energy; thus, any quench produces inverted mode occupation.

As discussed in the previous section, areas of zeros covering the real time axis result in jumps in the second time derivative of the dynamical free energy density if there is a jump in the density of zeros. Eq. \( \exists \bar{q} \) gives a “layer” of zeros for every \( n \in \mathbb{Z} \). Therefore, our total density of zeros is a sum of the densities of the individual “layers”, \( \rho(z) = \sum_n \rho^2_n(z) \). The single layer densities are given the Jacobi determinant of the change of variables \( \bar{k} \rightarrow z_n(\bar{k}) \).
\[\rho^N_n(z) = \frac{1}{\pi^2} \left| \frac{\partial \text{Re}(z_n)}{\partial k_x} \frac{\partial \text{Re}(z_n)}{\partial k_y} \right|^{-1} \]
\[= \frac{1}{\pi^2} \left[ \left( \frac{\partial_k B^2_k}{2E_k B_k^2} - \ln\left(\frac{B^2_k}{2E_k^2}\right) \partial_k E_k \right) - \left( \frac{\partial_k B^2_k}{2E_k B_k^2} - \ln\left(\frac{B^2_k}{2E_k^2}\right) \partial_k E_k \right) \right]^{-1} \]
\[= \frac{4E^2_k B^2_k}{(2n+1)\pi^3} \left( \partial_k E_k \partial_k E_k - \partial_k E_k \partial_k B_k^2 \right) \left( \frac{2n+1}{\pi} \right) \]
\[= \frac{4E^2_k B^2_k}{(2n+1)\pi^3} \left( \frac{\partial E_k}{\partial k} \frac{\partial E_k}{\partial k} - \frac{\partial E_k}{\partial k} \frac{\partial B_k^2}{\partial k} \right) \left( \frac{2n+1}{\pi} \right) \]
\[\tilde{k} \equiv \tilde{k}(z_n) \quad (39)\]

At this point a more technical view of the zeros of the partition function is useful: the zeros \(z_n(\tilde{k})\) correspond to intersections of the isolines
\[
B^2_k = \exp \left( \frac{(2n+1)\pi \text{Re}(z_n(\tilde{k}))}{\text{Im}(z_n(\tilde{k}))} \right),
\]
\[
E_k = \frac{(2n+1)\pi}{2\text{Im}(z_n(\tilde{k}))} \quad (40)
\]
in the momentum plane. This means that the density of zeros \(\rho^N_n(z)\) diverges at the boundary, since there \(\nabla E_k \parallel \nabla B^2_k\). Thus, when approaching the boundary of an interval \(T^*\) from the inside of the interval, the second time derivative of \(\text{Re}[f(t)]\) will diverge.

**IV. DYNAMICAL PHASE TRANSITIONS IN THE KITAEV HONEYCOMB MODEL**

**A. Zeros of the dynamical partition function in the Kitaev model**

In the Kitaev model not only quenches to the massless phase create inverted mode occupation. Also quenches across phase boundaries with final parameter \(J_f\) in a massive phase induce critical points in the real time evolution. It is physically reasonable to assume, that the mode occupation number \(\langle n_E \rangle\) is sufficiently well behaved, namely, that for any two \(\tilde{k}_0, \tilde{k}_1\) there exists a path \(\tilde{\gamma} : [0, 1] \to [-\pi, \pi]^2\) with \(\tilde{\gamma}(0) = \tilde{k}_0\) and \(\tilde{\gamma}(1) = \tilde{k}_1\) such that \(\langle n_{E(s)} \rangle, s \in [0, 1]\), is continuous. We found this to be true for all considered cases. Under this prerequisite, the existence of a fully occupied mode \(\tilde{k}^+\), \(\langle n_{E^+} \rangle = 1\), implies that \(\langle n_{E} \rangle = 1/2\) somewhere, because \(\langle n_{E^-} \rangle = 0\). \(\langle n_{E^+} \rangle = 1\) corresponds to \(|B_{E^+}| = \infty\) and this happens when
\[
0 = \epsilon_{E^+}(\tilde{J}_0) u_{E^+}(\tilde{J}_1) + v_{E^+}(\tilde{J}_0) v_{E^+}(\tilde{J}_1) \quad \wedge \quad 0 \neq u_{E^+}(\tilde{J}_0) v_{E^+}(\tilde{J}_1) - u_{E^+}(\tilde{J}_1) v_{E^+}(\tilde{J}_0) \quad (41)
\]

One possibility to fulfill this is
\[
\pm 1 = \frac{\epsilon_{E^+}(\tilde{J}_0)}{E_{E^+}(\tilde{J}_0)} = -\frac{\epsilon_{E^+}(\tilde{J}_1)}{E_{E^+}(\tilde{J}_1)} \quad (42)
\]

Now, consider a quench ending in the \(x\)-phase \((J^r_f \geq J^r_f + J^r_r)\) and \(\tilde{k}^+ = (\pi, 0)\). Then \(\epsilon_{E^+}(J_1) = 2(J^r_f - J^r_f + J^r_r)\) and \(\epsilon_{E^-}(J_1)/E_{E^+}(\tilde{J}_1) = -1\). We find that at this point both quenches, starting from another massive phase,
\[
J_0^y < J_0^y + J_0^y \Rightarrow \frac{\epsilon_{E^+}(\tilde{J}_0)}{E_{E^+}(\tilde{J}_0)} = 1 \quad (43)
\]
and from the massless phase,
\[
J_0^x < J_0^y + J_0^y \Rightarrow \frac{\epsilon_{E^+}(\tilde{J}_0)}{E_{E^+}(\tilde{J}_0)} = 1 \quad (44)
\]
lead to non-analytic behavior because (42) is fulfilled in both cases. The same can be shown for quenches ending in the other massive phases, only \(\tilde{k}^+\) needs to be chosen appropriately. This shows that in the Kitaev model occupation inversion is produced by quenches within the massless phase or quenches crossing phase boundaries.

Figure 4 displays locations of the zeros of the Loschmidt echo in the complex plane given by eq. (34) for two quenches, one within the \(A_x\) phase and one from the \(A_x\) phase to the massless phase. Both panels include a phase diagram with an arrow indicating the quench parameters \(J_0 \to J_1\). The numerical values for the parameters for this figure and all following figures are listed in Tab. III in the appendix. The zeros do indeed form areas, which are restricted to the left half-plane for the quench within the massive phase but cover parts of the real time (imaginary \(z\)) axis when \(J_0\) and \(J_1\) lie in different phases.

**B. Real time evolution**

On the real time axis the rate function of the Loschmidt echo \(L(t) = |Z(it)|^2\) reads
\[
r(t) = -\frac{1}{2\pi^2} \int_0^\pi \int_{-\pi}^\pi dk_x dk_y \ln \left( \frac{1 + 2B^2_k \cos(2E_k t) + B^4_k}{1 + B^2_k} \right) \quad (45)
\]
and the time derivative is
\[
\hat{r}(t) = \frac{1}{\pi^2} \int_0^\pi \int_{-\pi}^\pi \mathrm{d}k_x \mathrm{d}k_y \frac{B^2 E_k \sin(2E_k t)}{1 + 2B^2 E_k \cos(2E_k t) + B^2}.
\]

(46)

Figure 5 shows the time evolution of the rate function and its time derivative for various quenches obtained by numerical evaluation of the corresponding integrals. The gray-shaded areas indicate sections of the real time axis that are covered by areas of vanishing Loschmidt echo (cf. Fig. 4). If zeros of the Loschmidt echo cover parts of the time axis, also the density of zeros on the time axis, \( \rho_z(t) \), is included. Kinks in the time derivative of the rate function are observed when quenching across a phase boundary or within the massless phase.

spin chains. Let us consider the case \( J_z = 0 \). The vanishing of one of the other two parameters will give the same result due to the threefold symmetry. For \( J_z = 0 \) the condition for nonanalyticities (36) is fulfilled at \( \vec{q} \) with
\[
\cos(q_x - q_y) = \frac{J_x^0 J_y^1 + J_y^0 J_x^1}{J_x^0 J_y^1 + J_y^0 J_x^1}.
\]

(47)

Along this line also the spectrum is constant,
\[
E_{\vec{q}} = \sqrt{J_x^1 J_x^1 + J_y^1 J_y^1 + 2J_x^1 J_y^1 J_x^0 J_y^0 + J_x^0 J_y^1 + J_y^0 J_x^1}.
\]

(48)

Thus, the critical intervals \( T_n^* \) defined in eq. (36) become critical points
\[
t_n^* = \frac{(2n + 1)\pi}{2E_{\vec{q}}} = \frac{2n + 1}{2} t^*
\]

(49)
on the real time axis. Figure 6 shows the rate functions for two different quenches with \( J_y^0 = J_y^1 = 0 \). The quench in Fig. 6b does not cross a phase boundary and therefore the rate function is analytic. However, in Fig. 6a, \( \vec{J}_0 = (\frac{1}{2}, \frac{3}{2}, 0) \) and \( \vec{J}_1 = (\frac{1}{2}, 1, 0) \) lie in different phases, and according to eq. (49) there are critical

C. The 1d limit

In the limit \( J_\alpha \to 0 \) for any \( \alpha \in \{x, y, z\} \) the 2d Kitaev model (4) degenerates and becomes a set of separate 1d
times \( t_* = \frac{2n+1}{2} \sqrt{\frac{8}{\pi}} \) at which the rate function becomes singular. In particular, these singularities are discontinuities in the first time derivative of the rate function, not in the second as in the genuinely two-dimensional cases. This observation underlines the fact that the continuity of the first derivative is inherent to the higher dimensionality of the non-degenerate Kitaev model.

### D. The long time limit

In a recent work\cite{13}, it was stated that if the Loschmidt echo \( \mathcal{L}(t) \) supports analytic continuation, then the long real time limit \( \lim_{t \to \infty} \mathcal{L}(t) \) and the long imaginary time limit \( \lim_{t \to \infty} \mathcal{L}(-i\tau) \) coincide. In the context of dynamical phase transitions this gives rise to the conjecture, that the occurrence of DQPTs is closely related to the long time behaviour of \( \mathcal{L}(t) \). Dynamical quantum phase transitions occur if the zeros of the dynamical partition function cross the real time axis. This means, \( r(z) \), the rate function of the Loschmidt echo, is non-analytic in the \( \tau > 0 \) half plane; therefore, the long imaginary-time limit and the long real time limit do not necessarily have to coincide.

On the imaginary time axis \( z = \tau \), with the eigenbasis of the quenched Hamiltonian \( |\phi_n\rangle \), corresponding energies \( E_n \), and \( c_n = \langle \phi_n | \psi_i \rangle \),

\[
\mathcal{L}(-i\tau) = \left| \langle \psi_i | e^{-H \tau} | \psi_i \rangle \right|^2 = \left| \sum_{n,n'} c_n^* c_{n'} e^{-E_n \tau} \langle \phi_n | \phi_{n'} \rangle \right|^2 = \sum_n |c_n|^2 e^{-E_n \tau}.
\]

Now, shifting the energy such that \( E_0 = 0 \) and assuming the ground state \( |\phi_0\rangle \) to be non-degenerate,

\[
\lim_{\tau \to \infty} \mathcal{L}(-i\tau) = |c_n|^4 = |\langle \phi_0 | \psi_i \rangle|^4 = \mathcal{F}^4,
\]

where \( \mathcal{F} \equiv |\langle \phi_0 | \psi_i \rangle| \) is the fidelity. Thereby, the Loschmidt echo is connected to the fidelity in the large imaginary time limit.

As the Loschmidt echo is not well defined in the thermodynamic limit, one should rather formulate eq. \((51)\) in terms of the rate function:

\[
\lim_{\tau \to \infty} r(-i\tau) = -\lim_{\tau \to \infty} \lim_{N \to \infty} \frac{1}{N} \ln \mathcal{L}(-i\tau) = -\lim_{N \to \infty} \frac{1}{N} \ln \mathcal{F}^4
\]

According to the previous considerations this yields

\[
\lim_{t \to \infty} r(t) = -\lim_{N \to \infty} \frac{1}{N} \ln \mathcal{F}^4,
\]

if \( r(z) \) is analytic in the \( \tau > 0 \) half plane. This is a quite remarkable result: In the long time limit the Loschmidt echo approaches a value given solely by the overlap of the initial state with the ground state of the post-quench Hamiltonian, although the stationary state will surely never be that ground state. Quenching inevitably produces an excited state. Moreover, some information about the initial state is preserved for all times.

For the Kitaev model the fidelity is

\[
\mathcal{F} = \frac{|\langle 0 | \Pi_{\vec{k}} \left( 1 + B_{\vec{k}}^2 a_{\vec{k}} a_{-\vec{k}}^\dagger \right) | 0 \rangle|}{\sqrt{\langle \psi_0 | \psi_0 \rangle}} = \frac{1}{\sqrt{\langle \psi_0 | \psi_0 \rangle}} \exp \left( -\frac{N}{2} \sum_i \left( 1 + B_{\vec{k}}^2 \right) \right).
\]

Thus, if above conjecture is valid, we should find

\[
\lim_{t \to \infty} r(t) = \frac{1}{2\pi^2} \int d^2 k \ln \left( 1 + B_{\vec{k}}^2 \right)
\]

for quenches within the massive phases. Figure 7 shows the long time behavior of the rate function for a quench within the \( A_x \) phase and for a quench crossing phase boundaries; indeed, the rate function converges to the value given by the fidelity after the quench within the massive phase. In the other case, however, the rate function seems to converge, but the value it approaches differs from the one given by the fidelity. Various other cases were checked and the behavior was always consistent with above mentioned conjecture.

One can explain the convergence of the rate function heuristically based on the specific form given in eq. \((55)\). The expressions for the long time limit of the rate function in eq. \((55)\) and the definition of the rate function in eq. \((55)\) only differ in the nominators in the argument of the logarithm, which are \( 1 + B_{\vec{k}}^2 e^{-2i E_{\vec{k}} t} \), respectively. In the long-time limit the factor \( e^{-2i E_{\vec{k}} t} \) oscillates
also occur if the Hamiltonian parameter is continuously
that also slow ramping can produce a non-zero defect
the adiabatic theorem does not apply and it is known
in a gapless phase. In this case, the state of the system must at any time still be of the form
given in eq. (10), because at any time $H(\tilde{J}(t))$ can only excite both modes with opposite momenta $\vec{k}, -\vec{k}$ in one
$k$-sector. For $t > t_r$ the dynamics are the same as after a quench, however, the $B_{\vec{k}}$ will depend on the details of
the ramping protocol. As discussed above $B_{\vec{k}}$ is directly related to the mode occupation number $\langle n_{\vec{k}} \rangle$. Thus, in
order to determine, whether DQPTs occur after ramping from $\tilde{J}_0$ to $\tilde{J}_1$ instead of quenching, it is sufficient to
compute the mode occupation at $t = t_r$.

In order to get the mode occupation $\langle n_{\vec{k}} \rangle$ we make use of the fact that the total time evolution is simply made up
by the time evolution of independent two-level systems in the single $\vec{k}$-sectors and the corresponding Hamiltonians are

$$H_{\vec{k}}(\tilde{J}(t)) = \frac{1}{2} \left( \epsilon_{\vec{k}}(\tilde{J}(t)) \Delta_{\vec{k}}(\tilde{J}(t)) \right).$$

In these terms the initial state is the ground state of $H_{\vec{k}}(\tilde{J}_0)$.
$H_{\vec{k}}(\tilde{J}_0) \psi_{\vec{k},0} = -E_{\vec{k}}(\tilde{J}_0) \psi_{\vec{k},0}$, and the time evolved state $|\psi_{\vec{k}}(t)\rangle$ can be obtained by numerical in-
tegration of the Schrödinger equation. The mode occupation number after the ramping is then given by the overlap

$$\langle n_{\vec{k}} \rangle = |\langle \psi_{\vec{k}}^+ | \psi_{\vec{k}}(t_r) \rangle|^2,$$

where $H_{\vec{k}}(\tilde{J}_1) |\psi_{\vec{k}}^+\rangle = E_{\vec{k}} |\psi_{\vec{k}}^+\rangle$.

Figure 3 shows the occupation numbers for a quench within the gapless phase and for linear ramping with

$$\tilde{J}(t) = \begin{cases} \tilde{J}_0, & t < 0 \\ \tilde{J}_0 + (\tilde{J}_1 - \tilde{J}_0) t/t_r, & 0 \leq t \leq t_r \\ \tilde{J}_1, & t > t_r \end{cases}$$

and ramping period $t_r = 50$. As expected from the previous considerations the quench produces regions of non-
thermally occupied modes in the Brillouin-zone. Such areas are also present after the ramping. This means, that also in the time evolution for times $t > t_r$ there will be dynamical quantum phase transitions.

It is known that dynamical quantum phase transitions
also occur if the Hamiltonian parameter is continuously
ramped across a critical point instead of quenching it. However, it is not clear what happens after ramping the parameter within a gapless phase. In a gapless phase the adiabatic theorem does not apply and it is known
that also slow ramping can produce a non-zero defect density. But are these excitations sufficient to induce dynamical quantum phase transitions?

Assume the parameter $\tilde{J}(t)$ of the Hamiltonian is not
quenched immediately from $\tilde{J}(t < 0) = J_0$ to $\tilde{J}(t \geq 0) = J_1$, but continuously according to some protocol
with $\tilde{J}(t < 0) = J_0$ and $\tilde{J}(t > t_r) = J_1$. In this case, the
rate function converges in both cases.

E. Ramping

F. Quenching the magnetic field

In the presence of a magnetic field the phase $B$ (cf.
Fig. 2) becomes gapped and at $J_x = J_y = J_z \equiv J$
there exists a diagonal form of the Hamiltonian with
spectrum $E_{\vec{k}}(\tilde{J}, \kappa)$ as given in eq. (13), that maps to the

![Figure 7](image-url) Long-time behavior of the rate function (a) after a quench within the $A_x$ phase and (b) after a quench crossing phase boundaries. The rate function converges in both cases. For the quench within the massive phase it indeed approaches the value predicted by Heyl’s and Vojta’s conjecture (52), and in the other case the limit lies well off that value.
characterized by the Chern number \( \langle n_\mathbf{k}\rangle \) by such areas of zeros indicates the existence of critical points in the time evolution. We showed how this leads to dynamical quantum phase transitions as discontinuities in the second time derivative of the dynamical free energy as opposed to discontinuities in the first derivative known from 1d systems.

It was found that in the Kitaev honeycomb model dynamical quantum phase transitions occur after quenches across the phase boundaries and after quenches within the gapless phase. It is to our knowledge the first time that DQPTs are found in a two-dimensional model after quenching without crossing an equilibrium phase boundary. In accordance with the general considerations regarding the dynamics of BCS-type systems, DQPTs in the Kitaev model show up at the boundaries of the intervals \( T^n \) on the time axis which are included in a domain of zeros of the partition function. At these points the DQPTs appear as kinks in the first time derivative of the rate function of the Loschmidt echo. As was shown to hold for any BCS-type model, the curvature of the free energy density diverges when the boundary of such an interval is approached from the inward.

In degenerate versions of the Kitaev model, which effectively constitute one-dimensional spin chains, already the first derivative of the rate function becomes discontinuous after quenching across a phase boundary as known from other 1d models. This underlines the fact that the continuity of the first derivative is inherent to the higher dimensionality of the non-degenerate Kitaev model.

Moreover, we found for the Kitaev model that, in accordance with a conjecture concerning that matter, the long time stationary state of the rate function of the Loschmidt echo has a close connection to the occurrence of DQPTs: if no DQPTs occur, i.e., if the rate function is analytic in at least a half of the complex plane, the rate function approaches a value given by the fidelity. If the rate function is, however, non-analytic, it does in general point to discontinuities in the rate function of the Loschmidt echo. As was shown to hold for any BCS-type model, the curvature of the free energy density diverges when the boundary of such an interval is approached from the inward.
not converge to this value. The fact that the long time limit in absence of DQPTs is given by the fidelity deserves particular notice, since the fidelity is the overlap of the initial state with the ground state of the quenched Hamiltonian, but the approached stationary state is surely an excited state.

The examination of the mode occupation numbers after ramping the parameter of the Hamiltonian instead of quenching it implies that the subsequent time evolution also exhibits dynamical quantum phase transitions. Moreover, it was demonstrated that in the presence of a magnetic field quenches between the topologically ordered phases induce dynamical quantum phase transitions, which was previously proven to be a general feature in the dynamics of topologically ordered two-band models in Ref. [3].

DQPTs were to date not observed in experiments. The Loschmidt echo $L(t)$, which shows the non-analytic behavior, is not directly connected to a quantum mechanical observable. As mentioned above, the work density was suggested as an measurable quantity, which could show the signature of DQPTs. However, the Loschmidt echo becomes exponentially small with increasing system size, whereas, strictly speaking, DQPTs occur only in the thermodynamic limit. Experimentally measuring the signature of DQPTs in work densities will therefore be very challenging. Experimental consequences of DQPTs in other quantities than the work distribution function are currently being investigated. It was shown that DQPTs are connected to timescales of the order parameter dynamics in symmetry broken systems in particular the occurrence of DQPTs is directly related to the sudden transition from monotonous to oscillatory decay of the order parameter after a quench. Alternatively, the previously mentioned generalized expectation values could serve as measurable quantities. Moreover, it was shown in a recent work that DQPTs in Ising spin models exhibit scaling and universality and numerical results indicate that signatures of the DQPTs can be found in the dynamics of spin correlations as power-law scaling, which is solely determined by the universality class. This seems to provide a very promising opportunity for measuring DQPTs, since these quantities are accessible with current experimental techniques.

The finding of DQPTs as discontinuities in higher order derivatives in higher dimensional systems raises the question of a classification of dynamical quantum phase transitions. Canovi et al. suggested a formalism for such a classification. They related discontinuities in generalized expectation values and coexisting solutions to a first order transition. Here, we found a discontinuity in the second derivative of the dynamical free energy density. In future work it should be investigated how the findings of discontinuities in higher derivatives of the dynamical free energy density tie in with their definition.

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**Appendix A: Bogoliubov transformation and post-quench eigenbasis**

Consider the general Hamiltonian

$$H(\alpha) = \sum_{\vec{k}} \gamma_{\vec{k}} \left( \vec{b}_{\vec{k}}(\alpha) \cdot \vec{\sigma} \right) \gamma_{\vec{k}}$$

with $\vec{\sigma}$ the vector of Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and $\gamma_{\vec{k}}$ containing the creation and annihilation operators

$$\gamma_{\vec{k}} = \begin{pmatrix} d_{\vec{k}} \\ d_{-\vec{k}}^* \end{pmatrix}.$$

For $\alpha = \vec{J}$ and $\vec{b}_{\vec{J}}(\vec{J}) = (\Delta_{\vec{J}}(\vec{J})/2, 0, \epsilon_{\vec{J}}(\vec{J})/2)$ this gives the Hamiltonian of the Kitaev model as in eq. [4]. The unitary transformation

$$\begin{pmatrix} a_{\vec{k}}^2 \\ a_{\vec{k}}^{-1} \end{pmatrix} = W(\alpha) \gamma_{\vec{k}} = \begin{pmatrix} u_{\vec{k}}(\alpha) & v_{\vec{k}}(\alpha) \\ -v_{\vec{k}}(\alpha)^* & u_{\vec{k}}(\alpha)^* \end{pmatrix} \begin{pmatrix} d_{\vec{k}} \\ d_{-\vec{k}}^* \end{pmatrix}$$

(A4)

that brings the Hamiltonian (A1) into diagonal form is the Bogoliubov transformation. Plugging eq. (A4) into eq. (A1) and demanding that all off-diagonal terms vanish yields

$$0 = d_{\vec{k}}^x (u_{\vec{k}} v_{-\vec{k}} - u_{-\vec{k}} v_{\vec{k}}) + (d_{\vec{k}}^x - id_{\vec{k}}^y) u_{-\vec{k}} u_{\vec{k}} + (d_{\vec{k}}^x + id_{\vec{k}}^y) v_{-\vec{k}} v_{\vec{k}},$$

(A5)

where all the dependencies on $\alpha$ have been dropped for the sake of brevity. Since $W$ is unitary and $u_{\vec{k}}$ and $v_{\vec{k}}$ have the general form

$$u_{\vec{k}} = \cos \theta_{\vec{k}} e^{i\phi_{\vec{k}}}, \quad v_{\vec{k}} = \sin \theta_{\vec{k}} e^{i\phi_{\vec{k}}}.$$

(A6)

By choosing

$$\phi_{\vec{k}} = -\psi_{\vec{k}} = \frac{1}{2} \arctan \left( \frac{d_{\vec{k}}^y}{d_{\vec{k}}^x} \right)$$

(A7)

the equation above becomes real,

$$0 = d_{\vec{k}}^x \left( \sin \theta_{\vec{k}} \cos \theta_{\vec{k}} - \cos \theta_{-\vec{k}} \sin \theta_{\vec{k}} \right)$$

$$+ |d_{\vec{k}}^y| \left( \cos \theta_{\vec{k}} \cos \theta_{-\vec{k}} - \sin \theta_{\vec{k}} \sin \theta_{-\vec{k}} \right),$$

(A8)
where $d_{\vec{k}y}^x = d_{\vec{k}y}^x - id_{\vec{k}y}^x$ was introduced. Then for $a_{\vec{k}}^\dagger = (a_{-\vec{k}})^\dagger$ to hold, $\theta_{\vec{k}}$ must be an odd function of $\vec{k}$. Thus,

$$0 = -d_{\vec{k}}^z \sin(2\theta_{\vec{k}}) + |d_{\vec{k}}^z| \cos(2\theta_{\vec{k}})$$

$$\Rightarrow \tan(2\theta_{\vec{k}}) = \frac{|d_{\vec{k}}^z|}{d_{\vec{k}}^z}$$

(A9)

and this yields

$$|u_{\vec{k}}|^2 = \cos^2 \theta_{\vec{k}} = \frac{1}{2} \left( 1 + \frac{E_{\vec{k}}}{E_{\vec{k}}^*} \right)$$

$$|v_{\vec{k}}|^2 = \sin^2 \theta_{\vec{k}} = \frac{1}{2} \left( 1 - \frac{E_{\vec{k}}}{E_{\vec{k}}^*} \right).$$

(A10)

In the end it is left to choose the signs appropriately such that $u_{\vec{k}} = u_{-\vec{k}}$ and $v_{\vec{k}} = -v_{-\vec{k}}$, e.g.,

$$u_{\vec{k}} = e^{i\phi_{\vec{k}}} \sqrt{\frac{1}{2} \left( 1 + \frac{E_{\vec{k}}}{E_{\vec{k}}^*} \right)}$$

$$v_{\vec{k}} = \text{sign} \left( d_{\vec{k}}^z \right) e^{-i\phi_{\vec{k}}} \sqrt{\frac{1}{2} \left( 1 - \frac{E_{\vec{k}}}{E_{\vec{k}}^*} \right)}.$$  

(A11)

With this transformation the Hamiltonian (A1) becomes diagonal

$$H(\alpha) = \sum_{\vec{k}} \frac{E_{\vec{k}}(\alpha)}{2} \left( a_{\vec{k}}^\dagger a_{\vec{k}} - a_{-\vec{k}}^\dagger a_{-\vec{k}} \right)$$

(A12)

with $E_{\vec{k}}(\alpha) = |\vec{\delta}_{\vec{k}}(\alpha)|$.

To compute the quench dynamics one needs the connection of the degrees of freedom $a_{\vec{k}}^{\alpha_1}$ that diagonalise the initial Hamiltonian $H(\alpha_0)$ and the degrees of freedom $a_{\vec{k}}^{\alpha_1}$ diagonalising the final Hamiltonian $H(\alpha_1)$. This connection is given by two subsequent Bogoliubov transformations,

$$
\begin{pmatrix}
    a_{\vec{k}}^{\alpha_1} \\
    a_{-\vec{k}}^{\alpha_1}
\end{pmatrix}
= W(\alpha_1) W(\alpha_0)^\dagger
\begin{pmatrix}
    a_{\vec{k}}^{\alpha_0} \\
    a_{-\vec{k}}^{\alpha_0}
\end{pmatrix}
$$

$$= \begin{pmatrix}
    U_{\vec{k}}(\alpha_0, \alpha_1) & V_{\vec{k}}(\alpha_0, \alpha_1) \\
    -V_{\vec{k}}(\alpha_0, \alpha_1)^* & U_{\vec{k}}(\alpha_0, \alpha_1)^*
\end{pmatrix}
\begin{pmatrix}
    a_{\vec{k}}^{\alpha_0} \\
    a_{-\vec{k}}^{\alpha_0}
\end{pmatrix}
$$

(A13)

with

$$U_{\vec{k}}(\alpha_0, \alpha_1) = u_{\vec{k}}(\alpha_1) u_{\vec{k}}(\alpha_0)^* + v_{\vec{k}}(\vec{J}_1) v_{\vec{k}}(\alpha_0)^*$$

$$V_{\vec{k}}(\alpha_0, \alpha_1) = u_{\vec{k}}(\alpha_0) v_{\vec{k}}(\alpha_1) - u_{\vec{k}}(\alpha_1) v_{\vec{k}}(\alpha_0).$$

(A14)

Since $|\psi_i\rangle$ is the ground state of $H(\vec{J}_0)$

$$a_{\vec{k}}^{\alpha_0}|\psi_i\rangle = \left( U_{\vec{k}}(\alpha_0, \alpha_1) a_{\vec{k}}^{\alpha_1} - V_{\vec{k}}(\alpha_0, \alpha_1) a_{-\vec{k}}^{\alpha_1} \right) |\psi_i\rangle = 0$$

(A15)

must hold. Moreover, the ground state of a BCS-type Hamiltonian has vanishing total momentum; thus,

$$|\psi_i\rangle = \frac{1}{N} \prod_{\vec{k}} \left( 1 + B_{\vec{k}}(\alpha_0, \alpha_1) a_{\vec{k}}^{\alpha_1} a_{\vec{k}}^{\alpha_1 \dagger} \right) |0; \alpha_1\rangle$$

$$= \frac{1}{N} \exp \left( \sum_{\vec{k}} B_{\vec{k}}(\alpha_0, \alpha_1) a_{\vec{k}}^{\alpha_1} a_{\vec{k}}^{\alpha_1 \dagger} \right) |0; \alpha_1\rangle,$$

(A16)

where the coefficients $B_{\vec{k}}(\alpha_0, \alpha_1)$ are to be determined, $N$ is a normalization constant, and $|0; \alpha_1\rangle$ denotes the vacuum of the post-quench fermions: $a_{\vec{k}}^{\alpha_1}|0; \alpha_1\rangle = 0$. Plugging eq. (A16) into eq. (A15) yields

$$\left( U_{\vec{k}}(\alpha_0, \alpha_1) a_{\vec{k}}^{\alpha_1} - V_{\vec{k}}(\alpha_0, \alpha_1) a_{-\vec{k}}^{\alpha_1} \right) \prod_{\vec{k}} \left( 1 + B_{\vec{k}}(\alpha_0, \alpha_1) a_{\vec{k}}^{\alpha_1} a_{\vec{k}}^{\alpha_1 \dagger} \right) |0; \alpha_1\rangle$$

$$= \left( U_{\vec{k}}(\alpha_0, \alpha_1) B_{\vec{k}}(\alpha_0, \alpha_1) - V_{\vec{k}}(\alpha_0, \alpha_1) \right) a_{\vec{k}}^{\alpha_1} \prod_{\vec{k} \neq \vec{k}} \left( 1 + B_{\vec{k}}(\alpha_0, \alpha_1) a_{\vec{k}}^{\alpha_1} a_{\vec{k}}^{\alpha_1 \dagger} \right) |0; \alpha_1\rangle$$

$$= 0,$$

(A17)

which holds for

$$B_{\vec{k}}(\alpha_0, \alpha_1) = \frac{V_{\vec{k}}(\alpha_0, \alpha_1)}{U_{\vec{k}}(\alpha_0, \alpha_1)}$$

$$= \frac{u_{\vec{k}}(\alpha_0) v_{\vec{k}}(\alpha_1) - u_{\vec{k}}(\alpha_1) v_{\vec{k}}(\alpha_0)}{u_{\vec{k}}(\alpha_0) u_{\vec{k}}(\alpha_1) + v_{\vec{k}}(\alpha_0) v_{\vec{k}}(\alpha_1)}.$$  

(A18)

**Appendix B: Condition for real time zeros of the partition function**

The condition $B_{\vec{k}}^2 = 1$ (cf. eq. (35)) can be rearranged as follows: We have
\[
1 = |B_\epsilon|
\]
\[
\Leftrightarrow \left[ 1 + \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right] \left[ 1 + \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} + \text{sign}(\Delta_\epsilon(J_0)\Delta_\epsilon(J_1)) \right] \left[ 1 - \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right] \left[ 1 - \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} \right]
\]
\[
= \text{sign}(\Delta_\epsilon(J_1)) \left[ 1 + \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right] \left[ 1 - \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} - \text{sign}(\Delta_\epsilon(J_0)) \right] \left[ 1 - \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right] \left[ 1 + \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} \right]
\]
\[
\Leftrightarrow \left( 1 + \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right) \left( 1 + \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} \right) + \left( 1 - \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right) \left( 1 - \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} \right)
\]
\[
+ 2\text{sign}(\Delta_\epsilon(J_0)\Delta_\epsilon(J_1)) \left[ \left( 1 - \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right)^2 \right] \left( 1 - \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} \right)^2
\]
\[
= \left( 1 + \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right) \left( 1 - \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} \right) + \left( 1 - \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right) \left( 1 + \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} \right)
\]
\[
- 2\text{sign}(\Delta_\epsilon(J_0)\Delta_\epsilon(J_1)) \left[ 1 - \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right] \left( 1 - \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} \right)^2
\]
\[
\Leftrightarrow \frac{\epsilon_\epsilon(J_0)\epsilon_\epsilon(J_1)}{E_\epsilon(J_0)E_\epsilon(J_1)} = -\text{sign}(\Delta_\epsilon(J_0)\Delta_\epsilon(J_1)) \left[ \left( 1 - \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right)^2 \right] \left( 1 - \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} \right)^2
\]
\[
\Rightarrow 1 = \left( \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right)^2 + \left( \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} \right)^2 \quad \text{(B1)}
\]

Plugging this into the second last line we find the additional condition

\[
\text{sign}(\Delta_\epsilon(J_0)\epsilon_\epsilon(J_0)) = -\text{sign}(\Delta_\epsilon(J_1)\epsilon_\epsilon(J_1)), \quad \text{(B2)}
\]

Plugging in \( E_\epsilon(J)^2 = \epsilon_\epsilon(J)^2 + \Delta_\epsilon(J)^2 \) yields

\[
1 = |B_\epsilon|^2 \Leftrightarrow \left[ 1 = \left( \frac{\epsilon_\epsilon(J_0)}{E_\epsilon(J_0)} \right)^2 + \left( \frac{\epsilon_\epsilon(J_1)}{E_\epsilon(J_1)} \right)^2 \right] \wedge -1 = \frac{\text{sign}(\epsilon_\epsilon(J_1)\Delta_\epsilon(J_1))}{\text{sign}(\epsilon_\epsilon(J_0)\Delta_\epsilon(J_0))} 
\]

\[
\text{(B3)}
\]

So, for the emergence of a non-analyticity at a given time \( t = t^* \) we get two (simplified) conditions:

\[
E_\epsilon(J_1) = \frac{(2n + 1)\pi}{2t^*} \equiv C^*_t, \quad \text{(B5)}
\]

\[
0 = \Delta_\epsilon(J_0)\Delta_\epsilon(J_1) + \epsilon_\epsilon(J_0)\epsilon_\epsilon(J_1) \quad \text{(B6)}
\]

Appendix C: Quench/ramping parameters

Plugging in \( E_\epsilon(J)^2 = \epsilon_\epsilon(J)^2 + \Delta_\epsilon(J)^2 \) yields

\[
1 = |B_\epsilon(J_0, J_1)| \Leftrightarrow \Delta_\epsilon(J_0)\Delta_\epsilon(J_1) + \epsilon_\epsilon(J_0)\epsilon_\epsilon(J_1) = 0. \quad \text{(B4)}
\]
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Table I: Summary of the quench parameters used for the figures in the main text.

| Figure | Jx0 | Jy0 | Jz0 | Jx1 | Jy1 | Jz1 | κ0 | κ1 |
|--------|-----|-----|-----|-----|-----|-----|-----|-----|
| 4a)    | 0.8 | 0.1 | 0.1 | 0.6 | 0.2 | 0.2 | 0   | 0   |
| 4b)    | 0.8 | 0.1 | 0.1 | 0.4 | 0.3 | 0.3 | 0   | 0   |
| 5a)    | 0.8 | 0.1 | 0.1 | 0.6 | 0.2 | 0.2 | 0   | 0   |
| 5b)    | 0.8 | 0.1 | 0.1 | 0.2 | 0.1 | 0.7 | 0   | 0   |
| 5c)    | 0.8 | 0.1 | 0.1 | 0.4 | 0.3 | 0.3 | 0   | 0   |
| 5d)    | 0.4 | 0.3 | 0.3 | 0.4 | 0.3 | 0.3 | 0   | 0   |
| 6a)    | 0.1 | 0.9 | 0.0  | 0.4 | 0.6 | 0.0 | 0   | 0   |
| 6b)    | 0.25 | 0.75 | 0.0 | 0.75 | 0.25 | 0.0 | 0   | 0   |
| 7a)    | 0.9 | 0.05 | 0.05 | 0.6 | 0.2 | 0.2 | 0   | 0   |
| 7b)    | 0.9 | 0.05 | 0.05 | 0.1 | 0.8 | 0.1 | 0   | 0   |
| 8a)    | 0.8 | 0.1 | 0.1 | 0.6 | 0.2 | 0.2 | 0   | 0   |
| 8b)    | 0.8 | 0.1 | 0.1 | 0.4 | 0.3 | 0.3 | 0   | 0   |
| 9a)    | 1/3 | 1/3 | 1/3 | 1/3 | 1/3 | 1/3 | 0.5 | 0.1 |
| 9b)    | 1/3 | 1/3 | 1/3 | 1/3 | 1/3 | 1/3 | 0.5 | -0.1 |

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1. M. Greiner, O. Mandel, T. Esslinger, T. Hänsch, and I. Bloch, Nature 415, 39 (2002).
2. T. Kinoshita, T. Wenger, and D. Weiss, Nature 440, 900 (2006).
3. M. Heyl, A. Polkovnikov, and S. Kehrein, Phys. Rev. Lett. 110, 135704 (2013).
4. G. E. Fisher, Lectures in Theoretical Physics, Lectures in Theoretical Physics: Lectures Delivered at the Summer Institute for Theoretical Physics, University of Colorado, Boulder, Vol. 7 (Interscience, 1965).
5. C. Karrasch and D. Schuricht, Phys. Rev. B 87, 195104 (2013).
6. J. Kriel, C. Karrasch, and S. Kehrein, Phys. Rev. B 90, 125106 (2014).
7. S. Vajna and B. Dóra, Phys. Rev. B 91, 155127 (2015).
8. E. Canovi, P. Werner, and M. Eckstein, Phys. Rev. Lett. 113, 265702 (2014).
9. M. Fagotti, arXiv:1308.0277v2 (2013).
10. S. Vajna and B. Dóra, Phys. Rev. B 89, 161105 (2014).
11. F. Andraschko and J. Sirker, Phys. Rev. B 89, 125120 (2014).
12. J. Budich and M. Heyl, arXiv:1504.05599v1 (2015).
13. M. Heyl and M. Vojta, arXiv:1310.6226v2 (2013).
14. A. Kitaev, Annals of Physics 321, 2 (2006).
15. H.-D. Chen and J. Hu, Phys. Rev. B 76, 193101 (2007).
16. H.-D. Chen and Z. Nussinov, Journal of Physics A: Mathematical and Theoretical 41, 075001 (2008).
17. Here, we choose αr = −1 (cf. Ref. 16), such that the result for the spectrum agrees with the result in Ref. 14.
18. To be precise one would have to decide how to deal with the kx = 0-axis; however, this will not play any role in the later calculations.
19. C. N. Yang and T. D. Lee, Phys. Rev. 87, 404 (1952).
20. I. Bena, M. Droz, and A. Lipowski, International Journal of Modern Physics B 19, 4269 (2005).
21. W. van Saarloos and D. Kurtze, Journal of Physics A: Mathematical and General 17, 1301 (1984).
22. Assuming conventional continuity is too strong in this case, since in the Kitaev model the mode occupation number is not necessarily continuous after quenching (see Fig. S).
23. S. Mondal, D. Sen, and K. Sengupta, Phys. Rev. B 78, 045101 (2008).
24. M. Heyl, Phys. Rev. Lett. 113, 205701 (2014).
25. M. Heyl, arXiv:1505.02352v1 (2015).