Correlations and long-range mutual information in long-range Kitaev chains

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Long-range interactions exhibit surprising features which have been less explored so far. Here, studying a one-dimensional fermionic chain with long-range hopping and pairing, we discuss some general features associated to the presence of long-range entanglement. In particular, after determining the algebraic decays of the correlation functions, we prove that a long-range quantum mutual information exists if the exponent of the decay is not larger than one. Moreover, we show that the time evolution following from a quench between short-range and long-range regions, can be characterized by accidental dynamical quantum phase transitions. In conclusion, we discuss some topological features of the quantum phase, shedding light on the presence of zero Majorana fermions and the decay of their wave-functions, and the relation between the Kibble-Zurek mechanism and the divergence of a topological length scale at the topological quantum critical point.

I. INTRODUCTION

The study of the correlations between the parties of a many-body system in its quantum phases is a fundamental problem of condensed matter physics. A special role is played by the correlations that cannot be generated by local unitary evolutions, which give a so-called long-range entanglement [1]. In two dimensional systems, this leads to extraordinary topological phenomena, such as topological order with topological degeneracy of the quantum phase [2] and anyon excitations which can be employed in quantum fault-tolerant computation purposes [3], whose origin is revealed by topological entanglement entropy [4][5]. On the contrary, it is well known that the gapped quantum phases of one-dimensional systems can show only short-range entanglement if the interactions are short-ranged. Typically, for this kind of interactions, short-range and long-range entanglement regions are separated by an energy gap closing. Things change drastically when we consider long-range interactions. In this case, there is a path in the parameter space connecting short-range and long-range entanglement regions without closing the gap, also in one-dimensional systems. Moreover, the conventional topological classification [6][7] cannot be applied in the presence of long-range interactions, and new topological features emerge, like the presence of massive Dirac edge modes [8][9].

Here, we prove that the long-range entanglement in one-dimensional systems is intimately related to the algebraic decay of the correlation functions. In doing this, we characterize the long-range entanglement in the bulk by using the mutual information between two subsystems with sizes and separation which linearly increase with the size of the system. This quantity counts the total amount of correlations [10] and is an upper bound for squared correlation functions [11]. We find that it does not vanish in the thermodynamic limit if the correlation functions decay algebraically with an exponent not larger than one. We have discussed our results with the help of a specific model that is a chain of fermions with long-range hopping and pairing [9][12][13], which we have investigated thoroughly. The model displays long-range features including continuous quantum phase transitions without mass gap closure, violation of the area-law for the von Neumann entropy and emergence of massive edge states. For this model, we have calculated analytically the asymptotic formulas for the decay of the correlation functions. To make sure of the results, we have also characterized the long-range entanglement numerically by analyzing the largest Schmidt eigenvalue. Moreover, by considering the time evolution generated by a quench between short-range and long-range entanglement regions, we show that there are accidental dynamical quantum phase transitions [14][15]. Concerning the topological features of the model, we have discussed a general method, in the same spirit of Ref. [16], to study the existence and the decay of the wave functions of the zero Majorana fermions, which can acquire a mass becoming a complex Dirac fermion in the presence of long-range entanglement, and, in the end, we have shown how the Kibble-Zurek mechanism [17][18] is related to a topological scale length [19] of the quantum phase transition.

II. THE MODEL

We consider a chain of fermions described by the following Hamiltonian

\[
H = \frac{-W}{2} \sum_{j=1}^{L} \sum_{l=1}^{L-1} u_l(a_j^\dagger a_{j+l} + h.c.) - \mu \sum_{j=1}^{L} (n_j - \frac{1}{2})
+ \frac{\Delta}{2} \sum_{j=1}^{L-1} \sum_{l=1}^{L-j-1} v_l(a_j a_{j+l} + h.c.),
\]

where \(a_j\) (\(a_j^\dagger\)) annihilates (creates) a fermion in the site \(j\), \(w\) is the hopping amplitude, \(\mu\) is the chemical potential, \(\Delta\) is the superconductive pairing. We consider an algebraic decay of hopping and pairing interactions, so that for a closed chain (with periodic boundary conditions), we consider \(u_l = \theta(L/2-l)^{-\alpha} + \theta(l-1-L/2)(L-l)^{-\alpha}\) and \(v_l = \theta(L/2-l)^{-\beta} - \theta(l-1-L/2)(L-l)^{-\beta}\). For an open chain, the sum with respect to \(l\) runs from 1 to \(L-j\), and we consider \(u_l = 2l^{-\alpha}\) and \(v_l = 2l^{-\beta}\). In particular, in the limit \(\alpha \to \infty\) and \(\beta \to \infty\) we recover the conventional short-range Kitaev chain [20].

For a closed chain, we can perform a Fourier transform \(a_j = \frac{1}{\sqrt{L}} \sum_k e^{-ikj} a_k\), with \(k = 2\pi n/L, n = -(L-1)/2, \cdots , (L-1)/2\) for \(L\) odd, and \(n = -L/2 + 1, \cdots , L/2\) for \(L\) even. By defining the Nambu spinor \(\Psi_k = (a_k, a_{-k}^\dagger)^T\), the Hamiltonian...
reads
\[ H = \frac{1}{2} \sum_k \Psi_k^\dagger \left[ (\mu + wg(k)) \tau_3 + \Delta f(k) \tau_2 \right] \Psi_k, \tag{2} \]
where \( \tau_i \) with \( i = 1, 2, 3 \) are the Pauli matrices and where we defined the following functions \( g(k) = \sum_{l=1}^{L-1} u_l \cos(kl) \) and \( f(k) = \sum_{l=1}^{L-1} v_l \sin(kl) \). In the Majorana basis, \( \lambda_k = a_k + a_k^\dagger \), \( \lambda_k' = ia_k^\dagger - ia_k \), we get \( H = i/4 \sum_k \Lambda_k^T X(k) \Lambda_k \), with \( \Lambda_k = (\lambda_k, \lambda_k')^T \) and \( X(k) = i(\mu g(k) + \mu) \tau_2 - \Delta f(k) \tau_0 \), where \( \tau_0 \) is the identity matrix.

For short range interactions, the Majorana number \( \bar{g} \) indicates the presence of edge modes (if it is minus one) for the case of an open chain, and it is equal to \( \text{sign}((\mu + g(0)w)(\mu + g(\pi)w)) \). The proof is as follows: In order to evaluate the parity for \( L \) odd for a closed chain, we note that
\[ H = \frac{i}{4} \Lambda_k^T X(0) \Lambda_k + \frac{i}{4} \sum_{k=0}^{L-1} \left( \Lambda_k^T \Lambda_k \right) \left( X(-k) \right) \left( \Lambda_k \right) \tag{3} \]
We consider \( A = X(0) \oplus \left( \oplus_{k=0}^{L/2} \left( \begin{array}{cc} 0 & X(k) \\ X(-k) & 0 \end{array} \right) \right) \), then the parity is the sign of the Pfaffian of \( A \). Since \( \det X(k) > 0 \), by using the properties of the Pfaffian it is easy to show that \( \text{sign} PfA = \text{sign} PfX(0) = \text{sign}((\mu + g(0)w)) \). Similarly, for \( L \) even the parity is \( \text{sign} PfX(0) \oplus PfX(\pi) = \text{sign}((\mu + g(0)w)(\mu + g(\pi)w)) \), from which the expression of the Majorana number.

For an open chain, the quadratic Hamiltonian can be diagonalized with the general method reported in Ref. [21]. By performing a numerical investigation, we find that in the region where the Majorana number is \(-1\), there can be Majorana zero modes which can acquire a mass if \( \beta \) is small enough while they are massless if \( \beta > \min\{1, \alpha\} \), and their wave-functions become bi-localized at the edges, forming a non-local complex Dirac fermion.

For a closed chain, the Hamiltonian in Eq. (2) can be written as
\[ H = \sum_k \Psi_k^\dagger \delta_k \cdot \tau \Psi_k, \]
which, in the diagonal form, reads \( H = \sum_k \epsilon_k a_k^\dagger a_k \), obtained after performing a rotation with respect the \( x \)-axis with an angle \( \theta_k \) between \( \delta_k \) and the \( z \)-axis, corresponding to the Bogoliubov transformation \( a_k = \cos(\theta_k/2) a_k^\dagger - \sin(\theta_k/2) a_k^\dagger \), where \( \epsilon_k = 2||\delta_k|| = \sqrt{(\mu + wg(k))^2 + (\Delta f(k))^2} \). In the thermodynamic limit, the functions \( g(k) \) and \( f(k) \) can be written in terms of polylogarithms as \( g(k) = 2Re Li_\alpha(e^{ik}) \) and \( f(k) = 2Im Li_\beta(e^{ik}) \).

### III. Correlation Functions

In the thermodynamic limit, the correlation functions
\[ C_{ij} = \langle a_i^\dagger a_j \rangle, \quad F_{ij} = \langle a_i^\dagger a_j \rangle \]
which depend on the relative distance between \( i \) and \( j \), read
\[ C_R = \frac{\delta_{R,0}}{2} + \frac{1}{4i} \int_{|z|=1} dz \frac{(\mu + w(Li_\alpha(z) + Li_\alpha(1/z)))z^{R-1}}{\sqrt{(\mu + w(Li_\alpha(z) + Li_\alpha(1/z)))^2 - (\Delta(Li_\beta(z) - Li_\beta(1/z)))^2}}, \tag{7} \]
\[ F_R = \frac{1}{2} \int_{|z|=1} dz \frac{\Delta(Li_\beta(z) - Li_\beta(1/z))z^{R-1}}{\sqrt{(\mu + w(Li_\alpha(z) + Li_\alpha(1/z)))^2 - (\Delta(Li_\beta(z) - Li_\beta(1/z)))^2}}, \tag{8} \]
where the path of integration is drawn in Fig. [1]. By using the residue theorem, a pole \( z_0 \) of the integrand which is inside the unit circle gives an exponential decay \( z_0^R \), conversely, the brunch cut of the polylogarithm gives an algebraic decay, which goes as
\[ C_R \sim Im \int_0^{1} dx \frac{z^x}{\sqrt{(\mu + w(Li_\alpha(x) + i0^+) + Li_\alpha(1/x - i0^+)))x^{R-1}}}, \tag{9} \]
\[ F_R \sim Im \int_0^{1} dx \frac{\Delta(Li_\beta(x + i0^+) - Li_\beta(1/x - i0^+)))x^{R-1}}{\sqrt{(\mu + w(Li_\alpha(x + i0^+) + Li_\alpha(1/x - i0^+)))^2 - (\Delta(Li_\beta(x + i0^+) - Li_\beta(1/x - i0^+)))^2}}. \tag{10} \]

We note that as \( R \to \infty \), \( z_0^R \) is non zero only near one, thus we approximate the integrand with its expression near to one. For instance, if \( \beta < \min\{1, \alpha\} \), by considering an expansion of the polylogarithm near one, the term \( \Delta(Li_\beta(x + i0^+) - Li_\beta(1/x - i0^+)) \) in the denominator dominates, so that
we get $F_{R0} \sim \int_{0}^{1} x^{R-1}dx = R^{-1}$. Similarly, we can calculate the asymptotic formulas for the correlation functions in all the situations reported in Table I.

**TABLE I.** The exponents $a$ and $b$ of the algebraic decay of the correlation functions $C_{R0} \sim R^{-a}$ and $F_{R0} \sim R^{-b}$, for $a > 1$ and $a < 1$. Notice that for $a > 1$ and $\mu = -2\ln a(1)$ the exponents can be different, for instance we get $b = 1$ for any $\beta$.

| $a > 1$ | $b < 1$ | $\beta = 1$ | $1 < \beta < 2$ | $\beta > 2$ |
|---------|---------|-------------|-----------------|------------|
| $a$     | $2 - \beta$ | $2\beta - 1$ | $\beta + 1$    | $\beta$   |
| $b$     | $1$     | $1$         | $\beta$        | $\beta$   |

| $a < 1$ | $\beta < 1$ | $\beta = \alpha$ | $1 < \beta < 2$ | $\beta > 2$ |
|---------|-------------|-----------------|-----------------|------------|
| $a$     | $1 - \beta + \alpha$ | $2 - \beta$ | $1 + 2\beta - 2\alpha$ | $5 - \beta$ |
| $b$     | $1$         | $1$            | $\beta - \alpha$ | $4 - \beta$ |

**IV. LONG-RANGE ENTANGLEMENT**

We first recall that a state $|\Phi\rangle$ is short-range entangled if and only if there is a quantum circuit with a finite depth $U_{\text{circ}}^{f} \equiv U_{f}^{(M)} \cdots U_{f}^{(2)} U_{f}^{(1)}$, where $U_{f}^{(i)}$ is a piecewise local unitary with range $m$, such that $|\Phi\rangle = U_{\text{circ}}^{f} |\Phi_{0}\rangle$, where $|\Phi_{0}\rangle$ is a product state (see Ref. [11] for details). In this case, any site can be correlated only with the sites in a neighborhood smaller than $J = 2(Mm - M + 1)$. As a result, if we divide the chain into three blocks $A$, $B$ and $C$, with $C$ between $A$ and $B$ whose size $\ell_{AB} \geq J$, the reduced matrix for the sub-system $A \cup B$ is $\rho_{A:B} = \rho_{A} \otimes \rho_{B}$. This implies that if there is short-range entanglement, then there are no correlations between arbitrary parties $A$ and $B$ if their spatial separation $\ell_{AB}$ is large enough. Other useful quantities for characterizing the long-range entanglement are the entanglement spectrum and the entanglement entropy of a block $A$ with $\ell$ sites.

We recall that the eigenvalues $\lambda_{ij}^{A}$ (in non-increasing order) of the ground-state reduced density matrix $\rho_{A}$ of the block $A$, i.e., the square of the Schmidt coefficients, form the entanglement spectrum, and the entanglement entropy (the von Neumann entropy) can be expressed as $S_{A}(\ell) = -\sum_{i} \lambda_{ij}^{A} \ln \lambda_{ij}^{A}$. By considering short-range entanglement and the three blocks $A$, $B$ and $C$, one can show that (see, for instance, Ref. [22]) $|\Phi\rangle = \sum_{\alpha, \beta, \eta} \alpha_{\alpha\beta\eta} |\psi_{A}^{\alpha}\rangle |\psi_{B}^{\beta}\rangle |\psi_{C}^{\eta}\rangle$, with $1 \leq \alpha, \beta, \eta \leq D$, where $D = 2^\ell$ is the dimension of the Hilbert space of $C$. Then, there are maximum $D$ non-zero eigenvalues $\lambda_{ij}^{A}$, and the entanglement entropy is bounded by $S_{A} \leq \ln D$, where the bound does not depend on the size $\ell$ of the block $A$. We note that if there is a finite number of non-zero $\lambda_{ij}^{A}$ for any block $A$, then there is short-range entanglement (since the state is a matrix product state with finite dimensions [22]). To calculate the entanglement spectrum, as shown in Ref. [22], we note that the reduced density matrix of a block $A$ can be expressed as

$$\rho_{A} = e^{-\sum_{k} \zeta_{k}^{A} \epsilon_{k}^{A}} / Z_{A}$$

where $\epsilon_{k}^{A}$ are fermionic operators (linked to the original fermionic operators $a_{i}$ by a unitary transformation) and $\pm \tanh(\epsilon_{k}^{A}/2)$ are the eigenvalues of the matrix

$$
\begin{pmatrix}
2C_{A} - 1 & 2F_{A} \\
-2F_{A} & -2C_{A} + 1
\end{pmatrix}
$$

where $C_{A}$ and $F_{A}$ are correlation functions associated to the block $A$. Actually, $\tanh^{2}(\epsilon_{k}^{A}/2)$ are the eigenvalues of $(2C_{A} - I_{A} - 2F_{A})(2C_{A} - I_{A} + 2F_{A})$. Once obtained $\epsilon_{k}^{A}$ we can write the $2^{\ell}$ eigenvalues of Eq. (11)

$$
\lambda_{ij}^{A} = e^{-\sum_{k} \zeta_{k}^{A} \epsilon_{k}^{A}} / Z_{A},
$$

where $\zeta_{k}^{A} = 0$ and $Z_{A} = \prod_{k} (1 + e^{-\zeta_{k}^{A}})$. We note that the long-range entanglement can be fully characterized by the greater eigenvalue $\lambda_{ij}^{A} = 1/Z_{A}$. If $\lambda_{ij}^{A} \to 0$ when the block size $\ell$ tends to infinity, we get $S_{A}(\ell) \geq -\ln \lambda_{ij}^{A} \to \infty$, implying long-range entanglement. If there is a number $N_{A}$ of finite $\lambda_{ij}^{A}$, we get $N_{A} \to \infty$, if and only if $\lambda_{ij}^{A} \to 0$. If $\lambda_{ij}^{A} \to \infty$, then $N_{A}$ is finite so that there is a finite number of non-zero eigenvalues $\lambda_{ij}^{A}$, implying short-range entanglement. Actually, for our model, we find two distinct behaviors for $\lambda_{ij}^{A}$: either $\lambda_{ij}^{A} \sim c + c'\ell^{r}$, or $\lambda_{ij}^{A} \sim c'\ell^{-r}$, for large enough $\ell$ (see Fig. 2). To detect the long-range entanglement we looked at the Pearson correlation coefficient $p_{\ell_{A} \ell_{B} \ell_{C}}$ between the variables $\ln \lambda_{ij}^{A}$ and $\ln \ell$. This quantity tends to $-1$ in the presence of long-range entanglement. The Pearson correlation coefficient is defined as follows. Given two sets of variables $\{x_{1}, \cdots, x_{n}\}$ and $\{y_{1}, \cdots, y_{n}\}$, we define the Pearson correlation coefficient the quantity $p_{x,y} = \text{covar}(x,y) / \sqrt{\text{var}(x)\text{var}(y)}$, where $\text{covar}$ is the covariance and $\text{var}$ is the variance. As shown in Fig. 3 we observe long-range entanglement for $\beta \leq \min\{1, a\}$. Actually, we also find that, for $\beta \leq 1$, the exponent $\gamma$ appearing in the asymptotic behavior for the entanglement spectrum, $\lambda_{ij} \sim \ell^{-\gamma}$, saturates to the value $\gamma \approx 0.083 \approx 1/12$, (see Fig. 2 bottom panel) for $\beta \leq a$, extending the known result for the entanglement entropy for long-range paring [9,12,23], also in the presence of both long-range hopping and pairing terms, getting

$$
S_{A} = \frac{\text{const}}{6} \log \ell
$$
FIG. 2. (Top panel) Plot of $\lambda_1^{\alpha}$, as a function of the block size $\ell$ for $\beta = 1$ (red dots) and $\beta = 1.2$ (blue dots). We put $w = \Delta = 1$, $\mu = 0$ and $\alpha \to \infty$. The blue line is the best fit with the function $c + c'e^{-\gamma}$, where $c \approx 0.441$, $c' \approx 0.17$, and $\gamma \approx 0.471$, while the red line is the best fit with the function $c' e^{-\gamma}$, where $c' \approx 0.546$ and $\gamma \approx 0.052$ (the best fits have been performed for $\ell \geq 1000$). (Bottom panel) Plot of $y = c_{\text{eff}}/6$ as a function of $\beta$ for different values of $\alpha$ (obtained by best fitting in the interval $\ell \in [1000, 2000]$). For small $\beta$ and such that $\beta < \min\{1, \alpha\}$, the value of $y$ approaches $0.083 \approx 1/12$.

where the effective central charge reads $c_{\text{eff}} = 6\gamma \approx 0.5$, for $\beta \leq \min\{1, \alpha\}$.

FIG. 3. Plot of $e \equiv (\rho_{\ell \ell_i} \ln \lambda_i^{\alpha} + 1)$, namely the Pearson correlation coefficient plus one, in the $\alpha$-$\beta$ plane. We put $w = \Delta = 1$, $\mu = 0$. To calculate $e$, we considered the interval $\ell \in [300, 2000]$ by changing $\ell$ by steps of 100, and we calculated $\lambda_i^{\alpha}$ at the values $\alpha = 0.2 + 0.2 \times n$ and $\beta = 0.2 + 0.2 \times n$ with $n = 0, 1, \ldots, 7$. We verified in this way that, for $\beta \leq \min\{1, \alpha\}$, in the red region, $\lambda_i^{\alpha} \sim e^{-\gamma}$, for large enough $\ell$.

It is worth observing that the presence of long-range entanglement is related to the decay of correlation functions. To explain this relation, we consider a closed chain of $L$ sites and two blocks $A$ and $B$ of sizes $L_A = L_B = \ell = xL$, separated by a distance $\ell_{AB} = yL$, with $x$ and $y$ some fraction of $L$. To calculate the reduced density matrix $\rho_{AB}$ of the two blocks, it is useful to introduce the Majorana operators $c_{2j-1} = a_j + \alpha_j^\dagger$ and $c_{2j} = \alpha_j^\dagger - a_j$, and since their products form a basis in the operator linear space, we can make the ansatz

$$\rho_{AB} = \rho_A \otimes \rho_B + \frac{1}{2^{L_2}} \sum \delta \epsilon_l O_l,$$

where the sum is over all the possible products $O_l$ of an even number $n_l$ of Majorana operators belonging to both blocks $A$ and $B$, e.g., $\rho_{AB} = \rho_A \otimes \rho_B - \frac{1}{2^{L_2}} \left( \sum_{m \in A, n \in B} \epsilon mn \epsilon mv \epsilon mn' \epsilon mv' \ldots \right)$ and the quantities $\epsilon_l$ can be achieved by calculating the expectation values of $O_l$, so that we get, for instance, $\epsilon mn = \langle \epsilon mn \rangle$, $\epsilon mn' = \langle \epsilon mn \epsilon mn' \rangle$, and so on. If the correlation function $F_{20}$ dominates over $c_{\text{cor}}$ for large $R$, as $L \to \infty$, the term proportional to $\epsilon mn$ vanishes as $L \to \infty$, otherwise $\epsilon mn' \to L^{-2b}$, and it is easy to show that $\rho_{AB} \sim \rho_A \otimes \rho_B - \frac{1}{2^{L_2}} \sum_{i \in A, j \in B} F_{ij}(a_i a_j + a_j^\dagger a_i^\dagger)$. To study the scaling with the size $L$, it is enough to consider

$$\rho_{AB} \sim \rho_A \otimes \rho_B - \frac{\epsilon}{2^{L_2}} \sum_{i \in A, j \in B} (a_i a_j + a_j^\dagger a_i^\dagger),$$

where $\epsilon \sim \epsilon_{AB}^{b} \sim L^{-2b}$. For simplicity, we consider the trivial case $\rho_A \otimes \rho_B \propto I_{AB}$, by performing the transformation $a_i \to a_i^\dagger$ for $i \in A$, we get $\rho_{AB} \sim \exp(-\epsilon \sum_{i,j} a_i^\dagger J_{ij} a_j)$, with $J_{ij} = 1$ if $i \in A$ and $j \in B$, or $i \in B$ and $j \in A$. To characterize the correlation between the two parties $A$ and $B$, we consider the mutual information defined as

$$I_{AB} = S_A + S_B - S_{AB},$$

where $S_{AB}$ is the von Neumann entropy of the blocks $A$ and $B$, and so on. The entropy $S_{AB}$ can be expressed in terms of the eigenvalues $x_i$ of the matrix $J$ as $S_{AB} = \sum_i x_i (1 + e^{-x_i}) + \ln(1 + e^{-x_i})$, since there are only two non-zero eigenvalues $x_i$, which are $\pm(2xL)$, for $b > 1$, $xL \to 0$ and we get $S_{AB} \sim (2xL)(\ln 2 - 2 \epsilon (xL)^2)$. Concerning the mutual information, we have $I_{AB} \sim L^2 \epsilon^2 \sim L^{1-b}$, which tends to zero as $L \to \infty$ since $b > 1$. However, if $b \leq 1$, $I_{AB}$ does not vanish as $L \to \infty$, so that we have long-range entanglement in this case. In our case, looking at Table I we have at most $b = 1$ therefore we expect that, in those cases which correspond to $\beta \leq \min\{1, \alpha\}$, $I_{AB}$ saturates to a constant value in the limit of large system size, $L \to \infty$. We note that this result is quite general, i.e., does not depend on the choice of $\rho_A \otimes \rho_B$. To prove it, let us consider a general $\rho_{AB}$, not necessarily of the form of Eq. (15), and the eigenvalue equations $\rho_{AB} |\lambda_i^{AB}\rangle = \lambda_i^{AB} |\lambda_i^{AB}\rangle$, a similar equation for $B$, and $\rho_{AB} |\lambda_{ij}^{AB}\rangle = \lambda_{ij}^{AB} |\lambda_{ij}^{AB}\rangle$, with $\lambda_i^{AB} = \lambda_i^A \lambda_j^B + \delta \lambda_{ij}$, and $\delta \lambda_{ij}$ small enough, so that

$$I_{AB} \sim \sum_{ij} \delta \lambda_{ij} \ln(\lambda_i^{AB} \lambda_j^{AB}) + \sum_{ij} \frac{(\delta \lambda_{ij})^2}{2 \lambda_i^{AB} \lambda_j^{AB}}.$$
To guess the scaling of $\delta \lambda_{ij}$, let us consider for a moment $\rho_{AB}$ of the form of Eq. [15] and $\rho_A \otimes \rho_B \sim I_{AB}$. For the case $b \geq 1$, we have $\lambda_A^i \sim 2^{-L}$, and $\lambda_B^j \sim 2^{-L}$, since $\lambda_{ij} = 0$, by assuming $\delta \lambda_{ij} \sim \delta \lambda$, we get $\delta \lambda \sim \lambda_1^i \lambda_1^j \ell L$. Similarly, for $b \leq 1$, we get $\delta \lambda \sim \lambda_1^i \lambda_1^j$. In general, if $\lambda_A^i \sim \lambda_1^i$ and $\lambda_B^j \sim \lambda_1^j$, we assume that the relation $\delta \lambda \sim \lambda_1^i \lambda_1^j (L\delta)^\alpha$ holds also for generic $\rho_A \otimes \rho_B$. In particular, for $b \leq 1$ one can expect $\delta = 0$ and for $b > 1$ we have verified this hypothesis numerically in our model for the largest eigenvalue $\lambda_1^{AB} = \lambda_1^i \lambda_1^j$ and $\alpha > 1$ and $\beta > 1$ finding $\delta = 2$ (see Fig. 3). Then, if the hypothesis $B$ two simply connected partitions of the chain separated by a large distance, then $\rho_{A|B} \sim \rho_A \otimes \rho_B$. In that case the mutual information $I_{AB}$ of two disjoint and distant partitions is zero, as well as $S_D$. However, while for short-range interactions $S_D$ can be used as an order parameter for the topological phases, for long-range pairing, the long-range interactions leads to the generation of long-range entanglement in the bulk states, as shown in Ref. [29]. In this case $S_D$ turns out to be finite in a wider range of chemical potential. In other words, the long-range couplings induces a sort of long-range entanglement in the bulk defined as the lack of a short-range one.

![FIG. 4. Plot of $\delta \lambda_{ij}/(\lambda_1^i \lambda_1^j)$ as a function of $L$, for different values of $b$, where $x = 1/4$, $y = (1 - 2x)/2$, $\alpha = 2$, $w = \Lambda = 1$, $\mu = 0$ and $\beta = 1.2, 1.3, 1.4$ (from top to bottom). The solid lines are obtained by calculating the best fit with a function proportional to $L^{2(b-1)}$, in the interval $L \in [1000, 3000]$, by changing $L$ by steps of 100.](image1.jpg)

![FIG. 5. Plot of $I_{AB}$ as a function of $L$, for different values of $b$, where $x = 1/4$, $y = (1 - 2x)/2$, $\alpha = 2$, $w = \Lambda = 1$, $\mu = 0$ and $\beta = 0.9, 1.1, 1.2$ (from top to bottom). The value $\beta = 1$ corresponds to the red line. The solid lines are obtained by performing an extrapolation, calculating the best fit in the interval $L \in [1000, 6000]$, by changing $L$ by steps of 100, with a function $a' L^{-\gamma'} + b'$ for $\beta \leq 1$ and $a' L^{-\gamma'}$ for $\beta > 1$.](image2.jpg)

Finally, let us give an alternative analytical argument to explain the behavior reported in Eq. [18], getting $\delta = 2$ as obtained numerically. Defining the matrices

$$C_{AB} = \begin{pmatrix} I - C_{AB} & F_{AB}^T \\ F_{AB} & C_{AB} \end{pmatrix},$$

where $C_{AB}$ and $F_{AB}$ are matrices in real space whose elements, $C_{ij}$, $F_{ij}$ are the two-point correlation functions, Eq. [3], where $i \in A$, $j \in B$ (where $A$ and $B$ can or cannot coincide). For a connected subsystem, $A = B$, of size $t$, the eigenvalues of $C_{AA}$, defined as in Eq. [19], are $n_k^A = \frac{1}{1 + 2\varepsilon_k^A}$ and $n_k^B = \frac{1}{1 + 2\varepsilon_k^B} = 1 - n_k^A$, where $\varepsilon_k^A$ are the eigenvalues of the effective Hamiltonian of the reduced density matrix, Eq. [11], which can be easily written as $\rho_A = \phi_k \begin{pmatrix} n_k^A & 0 \\ 0 & n_k^B \end{pmatrix}$. As a result, the corresponding entanglement entropy is given by $S_A = -\sum_k \left( n_k^A \log n_k^A + n_k^B \log n_k^B \right)$. Let us now consider a subsystem $A \cup B$, made by two disjoint segments, $A$ and $B$, and define

$$C_{A|B} = \begin{pmatrix} C_{AA} & C_{AB} \\ C_{BA} & C_{BB} \end{pmatrix}$$
where the four elements are the correlation matrices given by Eq. (19). In order to calculate $S_{AUB}$ we have to find the eigenvalues $n^{^{AUB}}$ of Eq. (20) solving the following equation

$$\det (C_{BB} - C_{BB}(C_{AA} - n^{^{AUB}}_1)_1 C_{AB} - n^{^{AUB}}_2) \times \det (C_{AA} - n^{^{AUB}}_1) = 0$$

(21)

For $C_{AA} = C_{BB}$ and $C_{AB} = C_{BA}$, all $2\ell \times 2\ell$ matrices, Eq. (21) reduces to

$$\det (C_{AA} - C_{BB} - n^{^{AUB}}) \det (C_{AA} + C_{BB} - n^{^{AUB}}) = 0$$

(22)

valid also for non-commuting $C_{AA}$ and $C_{AB}$. We reduce the problem to simply finding the eigenvalues of $(C_{AA} \pm C_{BB})$.

So far everything is exact and represents an alternative route with respect to that describe previously to calculate the entropies. Let us now define, for simplicity, $q = (k, \pm z)$, which can be enumerated from $1$ to $2\ell$, and the unitary transformation $U$ which diagonalizes $C_{AA}$, namely $U^\dagger C_{AA} U = D_A$ where $D_A$ is a $2\ell$ diagonal matrix whose nonvanishing elements are $n_k^A$. Let us suppose that the eigenvalues $n_k^A$ are distinct. If $C_{AB}$ can be considered as a perturbation of $C_{AA}$, the eigenvalues of Eq. (20) are, at first approximation,

$$n_k^{^{AUB}} = n_k^A \pm \delta n_k \approx n_k^A \pm U^\dagger C_{AB} U$$

(23)

We notice that in $C_{AA}$ the matrices $C_{AA}$ and $F_{AA}$ (previously called $C_A$ and $F_A$) are symmetric Toeplitz matrices (which almost commute with a matrix $J$ where all the elements are equal to one, if boundary terms can be neglected). In $C_{AB}$, the matrices $C_{AB}$ and $F_{AB}$, for very large distances $\ell_{AB}$ can be approximated as $C_{AB} \sim C_{AB}^0 J$ and $F_{AB} \sim F_{AB}^0 J$. For $b < a$, we have $F_{AB}$ dominating over $C_{AB}$ and we get $\delta n_k^A \approx F_{AB}^0 \sum_{i<j} U_{ij}^0 \sim F_{AB}^0 \eta_0$ where $0 \leq \eta \leq 1$, depending on how much $U$ is a sparse matrix. Let us calculate the entanglement entropy $S_{AUB} = - \sum_{q=1}^{2\ell} \left( n_k^{^{AUB}} \log n_k^{^{AUB}} + n_k^{^{AUB}} \log n_k^{^{AUB}} \right)$, getting

$$S_{AUB} \approx 2S_A - 2 \sum_{q=1}^{2\ell} (\delta n_k^A)^2$$

(24)

where in the first term we have exactly $S_A = \sum_{q=1}^{2\ell} n_k^A \log n_k^A$ while the second term is the mutual information at first approximation, which reads $I_{AB} \sim \delta_{AB}^2 \eta^2$. If either the size of the blocks and their distance are extensive, i.e. $\ell \propto L$ and $\ell_{AB} \propto L$, we have $I_{AB} \sim L^2 (\eta - b)$. Since $\eta$ is bounded, $\eta \approx 1$, the mutual information surely vanishes for $b > 0$. This result is consistent with the leading term in Eq. (13), with $\delta = 2$.

We argue that $\eta \approx 1$. The reasoning goes as follows. Let us consider, for simplicity (non-supercorrelation) case, so that we have simply $C_{AA} = C_A$, which is a symmetric Toeplitz matrix, and $C_{AB} = C_{AB} \sim \ell^{-1} J$. Supposing that $\ell$ is very large so that $C_{AA}$ can be confused with a matrix with periodic boundary condition, making, therefore, an error on the boundary terms which might become negligible for large sizes. Under this assumption the unitary transformation $U$ is the Fourier transform $U_{jk} \approx e^{\pm 2\pi i k j / L}$ and, therefore, $\delta n_k = \delta_{k0} \ell^{-\frac{1}{2}}$. As a result, $S_{AUB} \approx 2S(A) - 2(\delta n_0^2) / n_0$, namely $I_{AB} \sim \ell^{-2} \eta^2$, meaning that $\eta \approx 1$.

V. MAJORANA ZERO FERMIONS

The quantum phase of the model can display zero Majorana fermions, in particular at the symmetric point $\mu = 0$, $\Delta = w = \alpha = \beta$, the Majorana fermions $c_1$ and $c_2$ are decoupled. By writing $H = \sum_{m,n} c_m^\dagger \mathcal{H}_{mn} c_n$, where $i \mathcal{H}$ is the real and skew-symmetric matrix

$$\mathcal{H} = \sum_{i,j} |i\rangle \langle j| \otimes H_{ij} = \sum_{j} |j\rangle \langle j| \otimes H_0$$

$$+ \sum_{j} \sum_{l} |j\rangle \langle j + l| \otimes H_l + |j + l\rangle \langle j| \otimes (H_l^\dagger)$$

(25)

where $H_0$ and $H_l$ are the matrices $H_0 = \mu \delta_{2}/4$ and $H_l = w l^{-\alpha} \tau_2 / 4 + l^{-1} \eta_1 / 4$, at the symmetric point $\mu = 0$ and $|2L|$ are eigenvectors of $\mathcal{H}$ with zero eigenvalue, where the nth component of $|i\rangle$ is $(|i\rangle)_n = \delta_{n,i}$. In general, if there are zero Majorana fermions then there are two eigenvectors $|\psi_1\rangle$ and $|\psi_2\rangle$ of $\mathcal{H}$ with zero eigenvalue and localized at the edges, and their components give the wave-functions of the Majorana fermions. To derive a condition for the existence of zero Majorana fermions and study the decay of their wave-functions, we define the projectors $P = |1\rangle\langle 1| + |2L\rangle\langle 2L|$ and $Q = I - P$, so that a generic matrix, in our case $\mathcal{H}$, can be written in a block form as

$$\mathcal{H} = \begin{pmatrix} \mathcal{H}_P & \mathcal{H}_{PQ} \\ \mathcal{H}_{QP} & \mathcal{H}_Q \end{pmatrix}$$

(26)

where $\mathcal{H}_P$ is the block corresponding to the subspace of $P$, and so on. We consider the eigenvalue equation $\mathcal{H}|\psi\rangle = E|\psi\rangle$, from which we get $P(\mathcal{H} - E)|\psi\rangle = 0$, or equivalently $(\mathcal{H}_P - E_P)|\psi_P\rangle + \mathcal{H}_P|\psi_Q\rangle = 0$, and $Q(\mathcal{H} - E)|\psi\rangle = 0$, i.e., $\mathcal{H}_Q|\psi_P\rangle + \mathcal{H}_Q|\psi_0\rangle = 0$. By combining these two equations, for $E = 0$, we get that there are zero Majorana fermions if the $2 \times 2$ matrix

$$\Gamma_P = \frac{1}{\mathcal{H}_Q} \mathcal{H}_{QP}$$

(27)

tends to zero as $L \to \infty$, where we have considered $\mathcal{H}_P \to 0$ in this limit, and $\mathcal{H}_Q$ non-singular. The wave-function of the Majorana fermion in the bulk is obtained by

$$|\psi_Q\rangle = -\frac{1}{\mathcal{H}_Q} \mathcal{H}_{QP}$$

(28)

where $|\psi_P\rangle$ is a two-dimensional vector.

We note that the matrix $\mathcal{H}_Q$ has elements $(\mathcal{H}_Q)_{m,1} = H_{m+1,1}$ and $(\mathcal{H}_Q)_{m,2} = H_{m+1,2L}$, with $m = 1, \ldots, 2L - 2$.

It is easy to see that $(\mathcal{H}_Q)_{2\ell-1,1} = i(1 + \delta_{1,0}) / \mu (1 - \delta_{0,1})$, thus if $\alpha = \beta$ and $\Delta = w$, if $|\psi_P\rangle = (1, \ell)^T$, we get $(|\psi_Q\rangle)_i = \mu (\mathcal{H}_Q^{-1})_{i,1} (I \mathcal{H}_Q^{-1})_{2L-2,1}$. Thus, since $(\mathcal{H}_Q^{-1})_{2\ell-1,1} = 0$, it is enough to study the asymptotic behavior of $(\mathcal{H}_Q^{-1})_{2\ell,1}$. By performing a numerical investigation, we find that $(\mathcal{H}_Q^{-1})_{2\ell,1}$ can decay for certain values of the parameters, then there are zero Majorana fermions having wave functions with the
same decay of \( (H^{-1})_{2j,1} \). For other values of the parameters, \( (H^{-1})_{2j,1} \) does not decay, so that \( \Gamma_0 \neq 0 \) and there are no zero Majorana fermions. To perform an analytic study, we consider periodic boundary conditions, and we change basis by defining the vectors \( |k\rangle \) such that \( |j\rangle = \sum_k e^{-ikj} |k\rangle / \sqrt{L} \), so that we get \( H = \sum_k |k\rangle \langle k| \otimes \mathcal{H}_k \), where

\[
((H^{-1})_{Q})_{2j,1} = \frac{2}{\pi} \operatorname{Im} \int_{|z|=1} dz \frac{1}{\mu + w(L_{1a}(z) + L_{1b}(1/z)) + \Delta(L_{1b}(z) - L_{1b}(1/z))}.
\]

In particular, the decay of \( (H^{-1})_{2j,1} \) can be approximated with the one of \( (H^{-1})_{1j,1} \) if the off-diagonal terms \( \mathcal{H}_{Q} \) and \( \mathcal{H}_{QP} \) are negligible, i.e., if \( \mu = 0 \), \( \omega \approx \Delta \) and \( \alpha \approx \beta \). We note that for \( \Delta = w = \beta = \alpha \), the function \( L_{1b}(z) \) for \( |z| < 1 \) has no branch cut, and we get a purely exponential decay. Otherwise, for \( \alpha > 1 \) and \( \beta > 1 \), we get

\[
((H^{-1})_{Q})_{2j,1} \sim \int dx x^{-1/2} (-\ln x)^{-\min\{\alpha, \beta\}-1} j^{-\min\{\alpha, \beta\}},
\]

and for \( \alpha < 1 \) or \( \beta < 1 \), we get \( ((H^{-1})_{Q})_{2j,1} \sim j^{2-\min\{\alpha, \beta\}} \). We note that for \( \alpha > 1 \) and \( \beta > 1 \) the estimation of the decay is in agreement with Ref. [16].

VI. DYNAMICAL QUANTUM PHASE TRANSITIONS

We proceed our discussion by focusing on the dynamical features. We start considering the time evolution generated by a sudden quench of the Hamiltonian, i.e., at the initial time \( t_0 = 0 \) the initial state of the system \( |\psi(t_0)\rangle \) is the ground-state of the initial Hamiltonian \( H \), and then the Hamiltonian is suddenly changed to \( H' \) (with apostrophized parameters, e.g., \( \mu' \)), generating the time evolution. Dynamical quantum phase transitions occur at the Fisher times, when the so-called Loschmidt amplitude, defined as \( G(t) = \langle \psi(t_1)|e^{-iH(t-t_0)}|\psi(t_1)\rangle \), and in the thermodynamic limit, the free energy density is analytic in \( G(t)/L \) is non-analytic [14]. As shown in Ref. [30], the presence of dynamical phase transitions can be related to the topological features of the quantum phases. In general, there are dynamical phase transitions if there is at least a \( k \) such that \( \tilde{d}_k \cdot \tilde{d}_0 = 0 \), and this is the case if we cross a topological quantum critical point with the quench. However, for our model, there are accidental dynamical phase transitions also if we cross the boundary between short-range and long-range entanglement. To prove it, we note that in the thermodynamic limit we get \( \tilde{d}_x = -\operatorname{sign}(\mu +wg(\pi))\hat{e}_3 \), \( \tilde{d}_0 = \operatorname{sign}(\Delta)\hat{e}_2 \) if \( \beta < \min\{1, \alpha\} \) and \( \tilde{d}_0 = -\operatorname{sign}(\mu +wg(0))\hat{e}_3 \) if \( \beta > \min\{1, \alpha\} \). Thus, if the quench is from a long-range region to a short-range one, we get \( \tilde{d}_0 \cdot \tilde{d}_0 = 0 \), so that there are dynamical phase transitions at the Fisher times \( t_{\alpha} = (n-1/2)\pi / (\epsilon'_{\alpha}) \). Vice versa, if \( \beta' < \min\{1, \alpha'\} \), \( \epsilon'_{\alpha} \) diverges as \( k \to 0 \), and \( t_{\alpha}'s \) are dense in \((0, \infty)\), so that the non-analytic behavior occurs at any time, \( \mathcal{H}_k = ((\mu +wg(k))\tau_2 - \Delta f(k)\tau_1) / 4 \). The inverse of the matrix \( \mathcal{H} \) reads

\[
\mathcal{H}^{-1} = -\frac{4i}{\pi} \int_0^{\pi/2} d\phi \left( \begin{array}{cc} 0 & 1/X_+ \\ -1/X_- & 0 \end{array} \right),
\]

where \( X_\pm = \mu + wg(k) \pm i\Delta f(k) \). Then, for the block correspondent to the subspace of \( Q \), we get

\[
\mathcal{H}^{-1} = -\frac{4i}{\pi} \int_0^{\pi/2} d\phi \left( \begin{array}{cc} 0 & 1/X_+ \\ -1/X_- & 0 \end{array} \right),
\]

i.e., the free energy density is nowhere analytic in the complex plane.

VII. KIBBLE-ZUREK MECHANISM

We conclude our discussion by investigating how the density of adiabatic excitations, generated by crossing linearly in time a topological quantum critical point, is related to the topological features of the quantum phase transition. We start considering a chemical potential which changes linearly in time as \( \mu(t) = t/t_Q \) for \( t \in (-\infty, 0) \), such that we cross the quantum critical point \( \mu_c = -wg(0) \) for \( \beta > 1 \) (thus we consider \( \alpha > 1 \) in order to have a finite value for \( \mu_c \)). At the initial time \( t = -\infty \), the initial state is the state \( |\psi(-\infty)\rangle \) defined such that \( a_k^\dagger |\psi(-\infty)\rangle = 0 \) for any \( k \). At the final time \( t = 0 \), we get \( \mu(0) = 0 \) and the Hamiltonian can be expressed as \( H = \sum_k \epsilon_k \alpha_k^\dagger \alpha_k \). The state at the final time is \( |\psi(0)\rangle \), and we focus on the excitations probability \( p_k = \langle \psi(0)|a_k^\dagger \alpha_k|\psi(0)\rangle \), and the excitations density \( n = \int_0^{\pi} dk p_k / \pi. \) This can be calculated by using the time-dependent Bogoliubov method (e.g., see Ref. [31]), from which we get Landau-Zener differential equations. For \( \beta > 1 \) the gap closes at \( k = 0 \) and only large wavelengths contribute for which we get \( p_k \sim \exp(-\pi t_Q (\Delta f(k))^2) \), so that, if \( 1 < \beta < 2 \), \( f(k) \sim k^\beta - 1 \) as \( k \to 0 \) and we get \( n \sim \tau_Q / (2\beta^2) \); and if \( \beta > 2 \), \( f(k) \sim k \) and \( n \sim 1/\sqrt{t_Q} \), in agreement with Ref. [32]. By considering the Kibble-Zurek mechanism [13], if the so-called healing length goes like \( \xi \sim |\mu - \mu_c|^{-\nu} \) and the gap closes as \( E_{gap} \sim |\mu - \mu_c|^{\nu} \), so that the relaxation time is \( \tau_{rel} \sim 1/E_{gap} \), we expect the density of defects \( n \sim t_Q^{-1/(1+\nu)} \). In our case, the gap closes with \( \nu = 1 \), thus we expect \( \nu = 1 \) for \( \beta > 2 \) and \( v = 1/(\beta - 1) \) for \( 1 < \beta < 2 \). Conversely, by considering \( \mu(t) = -t/t_Q \) for \( t \in (-\infty, 0) \), so that we cross the quantum phase transition point \( \mu_c = -wg(\pi) \), we have a contribution only for \( k \) near \( \pi \), otherwise the tunnelling is negligible. Since \( f(k) \sim (k - \pi) \) as \( k \to \pi \), we get \( n \sim 1/\sqrt{t_Q} \) for any \( \alpha \) and \( \beta \), and from the Kibble-Zurek theory we expect \( v = 1 \). It is interesting to observe that the values of the exponent \( v \) are the same of the one of the characteristic length scale \( \xi \) related to the topological phase transition, which is defined by considering the
winding number

\[ W = \frac{1}{2\pi} \int_{-\pi}^{\pi} \partial_k \theta_k dk \]  

(31)

where \( \theta_k = \arcsin(\Delta f(k)/(\epsilon_k)) \), such that (see, e.g., Ref. [19])

\[ \int_{-\xi^{-1}}^{\xi^{-1}} \partial_k \theta_{k_0+k} dk = O(1) \]  

(32)

where \( \partial_k \theta_{k_0+k} \) can be approximated by the Taylor expansion for \( k \sim 0 \). For instance, for \( \mu = -wg(0) \) and \( 1 < \beta < 2 \), we get \( \partial_k \theta_k \sim |k|^{\beta-2}/(\mu + wg(0)) \) as \( k \rightarrow 0 \), thus by substituting in Eq. [32], by considering the principal value of the integral, we get \( \xi \sim |\mu + wg(0)|^{1/(1-\beta)} \).

VIII. CONCLUSIONS

We performed a complete study of the correlation functions for the Kitaev model with both long-range hopping and pairing finding all the analytical expressions for their algebraic asymptotic decays (see Table I). Moreover we find that the critical-like behavior of the entanglement entropy can be extended also in the presence of long-range hopping, as far as \( \beta < \min\{1, \alpha\} \). We investigated the condition for getting long-range mutual information shared by two extended disconnected regions. This quantity has to be finite in order to get a finite disconnected entanglement entropy which detects long-range entanglement entropy at the edges. We show that, deep in the long-range interacting regime, the mutual information between two generic segments is always finite even at infinite distances. This implies that the reduced density matrix of a composite subsystem cannot be factorized, getting a sort of long-range entanglement in the bulk. Looking at the time evolution generated by a quench between short-range and long-range entanglement regions, we show that there are accidental dynamical quantum phase transitions. Finally, we discussed a general method for detecting the existence and the decay of the wave functions of the zero Majorana fermions and shown how the Kibble-Zurek mechanism is related to a topological scale length of the quantum phase transition.

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