# Majorana edge states in Kitaev chains of the BDI symmetry class

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Majorana edge states in Kitaev chains possessing an effective time reversal symmetry with one fermionic site per unit cell are studied. It is found that for a semi-infinite chain the equations for the wave functions of Majorana zero modes can be reduced to a single Wiener-Hopf equation, for which an exact analytical solution exists. The obtained solution can be used to analyze the wave functions of Majorana modes in Kitaev chains with finite-range and infinite-range hopping and pairing on common footing. We determine the asymptotic behaviors of the wave functions at large distances from the edge of the chain for several infinite-range models described in the literature. For these models we also determine the asymptotic behavior of the energy of the fermionic state composed of two Majorana modes in the limit of long (finite) Kitaev chains.

## I. INTRODUCTION

Topological superconductors offer a promising platform for the implementation of a topological quantum computer [1, 2]. The simplest generic model of a topological superconductor has been proposed by Alexei Kitaev [3]. He considered a chain of spinless fermions with $p$-wave superconducting pairing – this model became famous as the Kitaev chain. Such chain with one fermionic site per unit cell is described by the Hamiltonian

$$\hat{\mathrm{H}} = \frac{1}{2}\sum_{l,n}\left[2t_{l-n}\hat{a}_l^\dagger \hat{a}_n + \Delta_{l-n}\hat{a}_l^\dagger \hat{a}_n^\dagger + \Delta_{l-n}^* \hat{a}_n \hat{a}_l\right]. \quad (1)$$

Here, the indices $n$ and $l$ number the fermionic sites, $t_l$ are hopping amplitudes, $\Delta_l$ are pairing amplitudes, the star $*$ denotes complex conjugation, $\hat{a}_l^\dagger$ and $\hat{a}_l$ are fermionic creation and annihilation operators, respectively: $\{\hat{a}_l, \hat{a}_n^\dagger\} = \delta_{ln}$, $\{\hat{a}_l, \hat{a}_n\} = 0$. The paring and hopping amplitudes satisfy the relations $t_{-l} = t_l^*$, $\Delta_{-l} = -\Delta_l$. Under certain conditions, a semi-infinite Kitaev chain ($l = 0, 1, 2...$) hosts a so-called Majorana zero mode (MZM) – a special kind of edge state with energy exactly equal to zero. In this case, the system is said to be a 1D topological superconductor. In a finite chain, MZMs appear at both ends of the chain, and they combine into an ordinary Bogoliubov quasiparticle possessing a near-zero energy $E_0$. MZMs are exemplary non-Abelian anyons, which are the key component of a topological quantum computer.

Despite the apparent artificiality of Kitaev's model, it had a huge impact on condensed matter physics and materials science. Kitaev's work has stimulated the experimental search of MZMs in quantum wires with induced effective $p$-wave pairing [4], and has inspired a vast amount of theoretical research. Most proposals for implementations of 1D topological superconductors are rather described by a continuous version of the Hamiltonian (1), however, some system based on atomic chains placed on superconductors have effective discrete Hamiltonians that are identical to (1) [5–7]. In such systems the spatial structure (probability density) of MZMs can be probed using scanning tunneling microscopy [8]. The Hamiltonian (1) and its 2D analog are also relevant for the description of cold atoms in optical lattices [9–12].

To determine the quasiparticle spectrum of the Kitaev chain, one should apply a Bogoliubov transformation that diagonalizes the Hamiltonian (1) [9]. This results in the following Bogoliubov-de Gennes (BdG) equations for quasiparticle wave functions $(u_l, v_l)^T$:

$$\sum_n \begin{pmatrix} t_{l-n} & \Delta_{l-n} \\ \Delta_{n-l}^* & -t_{n-l} \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix} = E \begin{pmatrix} u_l \\ v_l \end{pmatrix}, \quad (2)$$

where $E$ is the quasiparticle energy. To obtain the structure of an isolated MZM, we have to put $E = 0$ and consider a semi-infinite chain: $l, n = 0..\infty$. In the case of short-range hopping and pairing – $t_l = \Delta_l = 0$ for $|l| > 1$ – the MZM has been analyzed in detail by Kitaev [3], who found that its wave function falls off exponentially fast with distance from the chain edge. This result is valid for any model with finite-range couplings: one can prove this be seeking the solution of Eq. (2) in the form of a sum of exponentially decaying terms: $u_l, v_l \propto e^{-\lambda l}$ (possibly, with polynomial factors). Equation (2) within finite-range models also can be solved using the transfer-matrix approach [13, 14]. The situation changes drastically when infinite-range hopping or pairing is present. In particular, it has been demonstrated that in the case of a power-law falloff of hopping and pairing amplitudes – $\Delta_l, t_l \propto |l|^{-\alpha}$, $\alpha \geq 1$ – the MZM wave function also falls off in a power-law manner with increasing $l$ [5, 15–18].

Formally, Eq. (2) on a semi-infinite chain constitutes a vector Wiener-Hopf problem [19, 20]. To date, a general solution method for this problem is unknown even for two-component vectors. In practice, the wave functions of MZMs in chains with infinite-range couplings are determined numerically by solving Eq. (2) on a finite chain (unless a solution for a semi-infinite system can be guessed, like in Ref. [15]). However, it turns out that for a wide class of systems an exact analytical solution of our Wiener-Hopf problem can be obtained, which is demonstrated in the present work.

Let us consider the situation when Eq. (2) can be reduced to the real form, so that the coefficients $t_l$ and $\Delta_l$ are real. It is said then that the system possesses an effective time-reversal symmetry and belongs to the Altland-Zirnbauer class BDI [21–23]. If we put $E = 0$ in Eq. (2), we may find that the equations for $u_l + v_l$ and $u_l - v_l$ decouple. Thus, we obtain two scalar Wiener-Hopf equations, for which an exact analytical solution exists, as has been demonstrated by Gakhov [24]. The derivation of this solution is outlined in the present paper. The solution illustrates the bulk-boundary correspondence principle – the number of zero-energy edge states in a semi-infinite chain equals the modulus of the $\mathbb{Z}$ topological index which classifies the topological phases of the bulk. Using the explicit formulas for $u_l$ and $v_l$, we calculate the asymptotic behavior of these functions in the limit of large $l$ for several infinite-range models described in the literature with special focus on models with power-law falloff of pairing and hopping amplitudes.

A crucial characteristic of a Majorana qubit is the energy $E_0$ of the fermionic edge state composed of two MZMs. In finite Majorana wires (and Kitaev chains) this energy is generally non-zero, and it determines the characteristic time $\hbar/E_0$ during which a phase error occurs in an isolated qubit [3]. A part of the present paper is devoted to the discussion of the asymptotic behavior of the energy $E_0$ in the limit of long chains. We demonstrate how this behavior can be determined using the obtained asymptotics for the MZM wave functions.

The paper is organized as follows. In Sec. II, we derive the explicit analytical solution for the MZM wave functions in a semi-infinite chain. In Sec. III, we discuss chains with finite-range hopping and pairing. In Sec. IV, we consider some model Kitaev chains described in the literature and determine the numbers of MZMs and their asymptotic behaviors far from the chain edge. In Sec. V, the asymptotic behavior of the energy $E_0$ is analyzed in the limit of long (finite) Kitaev chains. In the conclusion, the main results are summarized. The appendices contain some technical details.

## II. GENERAL SOLUTION FOR MAJORANA EDGE MODES

Here and further we will consider the BdG equations (2) with real coefficients $t_l$ and $\Delta_l$. Let us calculate the wave functions of MZMs in a semi-infinite chain, such that $l, n = 0, 1, 2....$ If we put $E = 0$ and introduce a new set of unknown coefficients $s_l = u_l + v_l$ and $w_l = u_l - v_l$, we obtain the equations

$$\sum_{n=0}^{\infty}(t_{l-n} + \Delta_{l-n})s_n = 0, \tag{3}$$

$$\sum_{n=0}^{\infty}(t_{l-n} - \Delta_{l-n})w_n = 0. \tag{4}$$

Now we are dealing with scalar Wiener-Hopf equations. They can be solved using the method found by Gakhov [24], which is outlined below. For a special case, the method was previously described in Ref. [7]. Here, a more general and rigorous derivation is given.

For any square-summable solution of Eq. (3) we define its generating function $s(z)$:

$$s(z) = \sum_{l=0}^{+\infty} s_l z^l. \tag{5}$$

Generally, we know only that the series converges for $|z| < 1$. Let us define one more generating function:

$$Q(z) = \sum_{l=-\infty}^{+\infty} (t_l + \Delta_l) z^l. \tag{6}$$

For a start, we will assume that $t_l$ and $\Delta_l$ fall off exponentially fast with increasing $l$. Then, $Q(z)$ is regular in a ring $R_0 = \{z|\rho_1 < |z| < \rho_2\}$, where $\rho_1 < 1 < \rho_2$. We may note that the function $Q(z)$ defines the bulk spectrum of an infinite chain. Indeed, if we put in Eq. (2) $u_l, v_l \propto e^{ikl}$, where $k$ is a dimensionless quasi-wavenumber, we find the quasiparticle energies

$$E(k) = \pm \left|Q(e^{ik})\right|. \tag{7}$$

For the existence of localized zero-energy modes, the bulk spectrum must be gapped, i.e., $Q(z) \neq 0$ on the unit circle. Then, a ring $R = \{z|r_1 < |z| < r_2\}$ containing the unit circle exists, where both $Q(z)$ and $Q^{-1}(z)$ are regular. For $r_1 < |z| < 1$ the product $Q(z)s(z)$ is regular, and the series in Eqs. (5) and (6) can be multiplied in the standard way:

$$Q(z)s(z) = p(z), \tag{8}$$

where, due to Eq. (3), the series for $p(z)$ contains only negative powers of $z$:

$$p(z) = \sum_{l=-\infty}^{-1} p_l z^l. \tag{9}$$

It follows from this that $p(z)$ can be analytically continued to the region $|z| > r_1$. In the ring $R$ we have

$$s(z) = Q^{-1}(z)p(z), \tag{10}$$

so that $s(z)$ in our case is regular for $|z| < r_2$. Since $r_2 > 1$, this means that the coefficients $s_l$ fall off exponentially fast with increasing $l$ – this is the first non-trivial result that we obtain.

Now we will determine all functions $s(z)$ and $p(z)$ that satisfy Eq. (8) in the ring $R$. To solve this problem, we make use of the factorization [24]

$$Q(z) = Q_-(z)z^\kappa Q_+(z), \tag{11}$$

where $Q_+(z)$ and $Q_+^{-1}(z)$ are regular for $|z| \le r_2$, $Q_-(z)$ and $Q_-^{-1}(z)$ are regular for $|z| \ge r_1$ (including $z = \infty$), and $\kappa$ is an integer, which is called the Cauchy index (winding number) of $Q(z)$. It is given by

$$\kappa = \frac{1}{2\pi} \oint_{|z|=1} d(\arg Q(z)). \tag{12}$$

Note that $\kappa$ coincides up to sign with the winding number defined in Ref. [13], and thus it is the $\mathbb{Z}$ topological invariant of our system. The functions $Q_+(z)$ and $Q_-(z)$ can be taken in the form

$$Q_+(z) = \exp\left(\frac{1}{2\pi i} \oint_{|t|=1} \frac{\ln(Q(t)t^{-\kappa})}{t-z} dt\right) \tag{13}$$

for $|z| < 1$, and

$$Q_-(z) = \exp\left(-\frac{1}{2\pi i} \oint_{|t|=1} \frac{\ln(Q(t)t^{-\kappa})}{t-z} dt\right) \tag{14}$$

for $|z| > 1$. The choice of the branch of the logarithms does not matter here. In the ring $R$, the functions $Q_+(z)$ and $Q_-(z)$ are uniquely defined up to constant numerical factors.

From Eqs. (8) and (11) we obtain

$$Q_+(z)s(z) = z^{-\kappa} Q_-^{-1}(z)p(z). \tag{15}$$

Two cases are possible. If $\kappa \geq 0$, the Laurent series of the right-hand side of Eq. (15) contains only negative powers of $z$, while the Laurent series of the left-hand side contains only non-negative powers of $z$, which means that both sides must be equal to zero. We find then that $s(z) = 0$, and $s_l = 0$ for all $l$. The situation is different for $\kappa < 0$. We have then

$$Q_+(z)s(z) = P_{|\kappa|}(z) + \tilde{p}(z), \tag{16}$$

where

$$P_{|\kappa|}(z) = \sum_{m=0}^{|\kappa|-1} a_m z^m, \tag{17}$$

$a_m$ are some (arbitrary) constants, and the function $\tilde{p}(z)$ is a function whose Laurent series contains only negative powers of $z$. On the other hand, the Laurent series of $Q_+(z)s(z)$ contains only non-negative powers of $z$, which means that $\tilde{p}(z) = 0$, and

$$s(z) = Q_+^{-1}(z)P_{|\kappa|}(z). \tag{18}$$

The expansion coefficients of $s(z)$ are given by the relation

$$s_l = \frac{1}{2\pi i} \oint_{|z|=1} \frac{s(z)dz}{z^{l+1}} = \frac{1}{2\pi i} \oint_{|z|=1} \frac{P_{|\kappa|}(z)dz}{Q_+(z)z^{l+1}}. \tag{19}$$

We have demonstrated that any square-summable solution of Eq. (3) can be written in the form (19). On the other hand, we can do the calculations in reverse order to prove that any sequence $s_l$ given by Eq. (19) satisfies Eq. (3). Thus, Eq. (19) provides a general square-summable solution to Eq. (3). There are overall $|\kappa|$ linearly independent solutions for negative $\kappa$.

Equation (4) can be solved in a similar way. The difference is that we arrive at a relation similar to Eq. (8) with the function $Q(z^{-1})$ in the place of $Q(z)$. The Cauchy index of $Q(z^{-1})$ equals $-\kappa$. Hence, for $\kappa > 0$ Eq. (4) has $\kappa$ linearly independent solutions. Thus, we obtain $|\kappa|$ Majorana edge states in total.

To end this section, we briefly touch upon the case when a ring $R$ in the complex plane where $Q(z)$ is regular does not exist. This happens, e.g., when the coefficients $t_l$ and $\Delta_l$ exhibit a power-law decay with increasing $l$. Then, we redefine $Q(z)$ as follows:

$$Q(z) = \sum_{l=-\infty}^{+\infty} (t_l + \Delta_l) z^l e^{-\eta_+ |l|}, \tag{20}$$

where $\eta_+$ is positive. Then, all calculations following Eq. (6) can be reproduced. In the end, one has to go to the limit $\eta_+ \to 0$ to obtain the solutions of Eqs. (3) and (4). Of course, such extension of the Wiener-Hopf technique in not strictly justified, however, it seems reasonable as long as a limit for the Cauchy index exists when $\eta_+$ tends to zero.

## III. FINITE-RANGE HOPPING AND PAIRING

In this Section, we will analyze the solution of Eq. (3) in the case of finite-range hopping and pairing in the Kitaev chain, when $Q(z)$ is a polynomial. It can be written in the form

$$Q(z) = qz^{l_0} \prod_{j=1}^{N_-} \left(z - z_j^{(-)}\right) \prod_{j=1}^{N_+} \left(z - z_j^{(+)}\right), \tag{21}$$

where $l_0$ is an integer, $q$ is some constant, $z_j^{(-)}$ and $z_j^{(+)}$ are roots of $Q(z)$ such that $|z_j^{(-)}| < 1$ and $|z_j^{(+)}| > 1$ (the root $z = 0$ is not included in $z_j^{(-)}$), $N_-$ and $N_+$ are the numbers of roots of $z_j^{(-)}$ and $z_j^{(+)}$, respectively. The Cauchy index of $Q(z)$ is $\kappa = l_0 + N_-$, and the factors $Q_-$ and $Q_+$ can be taken in the form

$$Q_-(z) = q \prod_{j=1}^{N_-} \frac{\left(z - z_j^{(-)}\right)}{z}, \tag{22}$$

$$Q_+(z) = \prod_{j=1}^{N_+} \left(z - z_j^{(+)}\right). \tag{23}$$

We assume that $\kappa < 0$. Then, for sufficiently large $l$ Eq. (19) yields

$$s_l = -\sum_{j=1}^{N_+} \operatorname*{Res}_{z=z_j^{(+)}} \frac{P_{|\kappa|}(z)}{Q_+(z)z^{l+1}}. \tag{24}$$

If $Q_+(z)$ has only simple roots (the generalization for multiple roots is straightforward), we have

$$s_l = -\sum_{j=1}^{N_+} \frac{P_{|\kappa|}\left(z_j^{(+)}\right)}{Q'_+\left(z_j^{(+)}\right) z_j^{(+)l+1}}. \tag{25}$$

It can be seen that the asymptotic behavior of $s_l$ in the limit $l \to \infty$ is determined by the root $z_j^{(+)}$ with the smallest modulus (unless $P_{|\kappa|}(z_j^{(+)}) = 0$ for this root).

## IV. SOME MODELS WITH INFINITE-RANGE HOPPING AND PAIRING

### A. Power-law falloff of hopping pairing amplitudes with exponents larger than 1

In this Section, we will use the developed formalism to reconsider some model Kitaev chains studied in the literature. We start with the model studied in Refs. [14, 17, 18] with power-law falloff of pairing and hopping amplitudes:

$$t_l = \begin{cases} -\mu & \text{for } l = 0 \\ -\frac{J}{|l|^\alpha} & \text{for } l \neq 0 \end{cases}, \tag{26}$$

$$\Delta_l = \begin{cases} 0 & \text{for } l = 0 \\ \frac{\Delta}{|l|^\beta}\mathrm{sgn}(l) & \text{for } l \neq 0 \end{cases}, \tag{27}$$

where $\mu$, $\Delta$ and $J$ are constants. Note that Eqs. (26) and (27) formally encompass the cases of short-range hopping ($\alpha = \infty$) and pairing ($\beta = \infty$).

For a start, we confine ourselves to the case $\alpha > 1$ and $\beta > 1$, so that we can use Eq. (6) to define $Q(z)$ on the unit circle:

$$\begin{aligned} Q(z) = -\mu + \Delta\left[\mathrm{Li}_\beta(z) - \mathrm{Li}_\beta(z^{-1})\right] \\ -J\left[\mathrm{Li}_\alpha(z) + \mathrm{Li}_\alpha(z^{-1})\right], \end{aligned} \tag{28}$$

where $\mathrm{Li}_\gamma(z)$ is the polylogarithm:

$$\mathrm{Li}_\gamma(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^\gamma}. \tag{29}$$

It can can be demonstrated that the spectrum of an infinite chain is gapless as long as $Q(1) \neq 0$ and $Q(-1) \neq 0$, and that the Cauchy index equals (see Appendix A)

$$\kappa = \begin{cases} 0 & \text{when} \quad Q(1)Q(-1) > 0, \\ 1 & \text{when} \quad Q(1)\Delta > 0 \text{ and } Q(-1)\Delta < 0, \\ -1 & \text{when} \quad Q(-1)\Delta > 0 \text{ and } \quad Q(1)\Delta < 0. \end{cases} \tag{30}$$

Let us consider the special case when $\Delta = J$ and $\alpha = \beta$, so that $Q(z)$ takes the form

$$Q(z) = -\mu - 2J\mathrm{Li}_\alpha(z^{-1}). \tag{31}$$

This function is regular for $|z| > 1$ (including $z = \infty$), and hence $\kappa \leq 0$. We obtain $\kappa = -1$ when (compare with Ref. [14])

$$(\mu + 2J\zeta(\alpha))[\mu - 2J\zeta(\alpha)(1 - 2^{-\alpha})] < 0, \tag{32}$$

where $\zeta(x)$ is the Riemann zeta function. Then, $Q(z)$ has one real root $z = z_0$ in the region $|z| > 1$. If we substitute $Q_+(z) = Q_-^{-1}(z)Q(z)z$ in Eq. (19), we may find that the integral in this equation is determined by the residue of the integrand at $z = z_0$. This yields a solution for $s_l$ of the form $s_l = z_0^{-l}$ – it can be easily checked that this satisfies Eq. (3). If we take $\mu = 0$, we obtain $z_0 = \infty$, which results in a Majorana edge mode localized at the site $l = 0$ [18].

Now let us assume that either $\alpha \neq \beta$, or $\Delta \neq J$, and $\kappa = -1$. The asymptotic behavior of $s_l$ in the limit of large $l$ in this case is determined in Appendix A:

$$s_l \approx \mathrm{const}\left[\frac{\Delta}{l^\beta} - \frac{J}{l^\alpha}\right]. \tag{33}$$

This behavior is consistent with the one reported in Ref. [18] [25]. It should be noted though that the two terms in the right-hand side of Eq. (A10) do not necessarily represent the two main contributions to $s_l$, because the asymptotic expansion of $s_l$ also contains terms proportional to $l^{-\alpha-n}$ and $l^{-\beta-n}$ with $n \in \mathbb{N}$.

### B. Special case of inverse-distance falloff of pairing and hopping amplitudes

The cases when $\alpha$ or $\beta$ in Eqs. (26) and (27) are integers is somewhat special: then, Eq. (33) is not applicable. In particular, for $\gamma = 1$ one can see that Eq. (29) yields

$$\mathrm{Li}_1(z) = -\ln(1 - z). \tag{34}$$

Hence, if one considers pairing and hopping amplitudes with asyptotic behavior $t_l, \Delta_l \propto |l|^{-1}$, the function $Q(z)$ acquires logarithmic singularities on the unit circle. Particular examples of this have been analyzed by Pientka *et al.* [5, 15] and Bespalov [7], where pairing and hopping amplitudes were considered that exhibit oscillations together with a $|l|^{-1}$ falloff.

We will briefly review the results obtained for the more general model studied by Bespalov. Within this model, the function $Q(z)$ has the form

$$\begin{aligned} Q(z) = \epsilon - (\rho + 1)g^*\left[\mathrm{Li}_1(e^{i\varphi_1}z) + \mathrm{Li}_1(e^{i\varphi_2}z^{-1})\right] \\ +(1 - \rho)g\left[\mathrm{Li}_1(e^{i\varphi_2}z) + \mathrm{Li}_1(e^{i\varphi_1}z^{-1})\right] \\ +(1 - \rho)g^*\left[\mathrm{Li}_1(e^{-i\varphi_2}z) + \mathrm{Li}_1(e^{-i\varphi_1}z^{-1})\right] \\ -(\rho + 1)g\left[\mathrm{Li}_1(e^{-i\varphi_1}z) + \mathrm{Li}_1(e^{-i\varphi_2}z^{-1})\right], \end{aligned} \tag{35}$$

where $\epsilon$, $\rho$, $\varphi_1$ and $\varphi_2$ are real numbers, $0 < \rho \leq 1$, and $g$ is a complex number. Discrete BdG Hamiltonians characterized by such functions $Q(z)$ arise in the studies of quasiparticle excitations induced by helical magnetic atom chains in bulk superconductors ($\rho = 1$) and constriction-type Josephson junctions ($\rho \le 1$). The factorization of $Q(z)$ given by Eq. (35) is quite nontrivial. In particular, to determine the behavior of $Q_+(z)$ in the vicinity of its singularities, the right-hand side of Eq. (13) must be evaluated. This has been done in Ref. [7] in the case when none of the four singular points $e^{i\varphi_1}$, $e^{-i\varphi_1}$, $e^{i\varphi_2}$ and $e^{-i\varphi_2}$ coincides with the others. It was found that when the index $\kappa$ equals $-1$, the asymptotic behavior of $s_l$ in the limit of large $l$ is given by the formula

$$s_l \approx \frac{\cos(l\varphi_1+\beta_1)}{l(\ln l)^{\frac{3}{2}+\frac{1}{2\rho}}} + \frac{C\cos(l\varphi_2+\beta_2)}{l(\ln l)^{\frac{3}{2}-\frac{1}{2\rho}}}, \tag{36}$$

where $\beta_1$, $\beta_2$ and $C$ are real numbers that do not depend on $l$. For $\rho = 1$ the number $C$ vanishes, and we obtain $s_l \propto 1/(l\ln^2 l)$ [5, 15].

### C. Power-law falloff of pairing and hopping amplitudes with exponent smaller than 1

Let us now consider the case when either $\alpha < 1$ or $\beta < 1$ (or both). As discussed in the literature, there is an ambiguity in the definition of the winding number when $\beta \le \alpha$ and $\beta < 1$. It has been claimed that the winding number takes half-integer values, which is accompanied by the appearance of so-called massive Dirac edge states, which have a non-vanishing energy for any length of the Kitaev chain [14, 16, 17, 26, 27]. It has been even argued that in this case the ten-fold way classification of topological insulators and superconductors is not applicable, and that the bulk-boundary correspondence is weakened [28].

Let us consider this situation from the point of view of the Wiener-Hopf technique. When $\alpha < 1$ or $\beta < 1$, the function $Q(z)$ is discontinuous on the unit circle at $z = 1$, and we have to use Eq. (20) with $\eta_+ \to +0$ to construct a factorization given by Eq. (11). Let us assume that $\beta < \alpha$. Then, $Q(z)$ has a real root lying in the interval $(e^{-\eta_+}, e^{\eta_+})$. This root tends to 1 in the limit $\eta_+ \to 0$, which makes the winding number ill-defined in this limit. This corresponds to the "half-integer winding number" mentioned above. Then, the edge states have a non-vanishing energy even in long chains, and the developed above formalism does not allow to determine their wave functions.

The situation is different when $\alpha < \beta$. Then, the winding number is well-defined in the limit $\eta_+ \to 0$, and it can be calculated as described in Sec. IV A, assuming that $Q(1) = -\infty \cdot \mathrm{sgn}(J)$. As demonstrated in Appendix A, in the limit of large $l$ we again obtain a power-law falloff of the MZM wave function: $s_l \propto l^{(\alpha-3)/2}$.

In a similar way, the asymptotic behavior of $s_l$can be determined for $\alpha = \beta < 1$ and for $|J| > |\Delta|$: $s_l \propto l^{-1-\chi}$, where

$$\chi = \pi^{-1}\,\mathrm{arccot}\left(\frac{J-\Delta-(\Delta+J)\cos(\pi\alpha)}{(J+\Delta)\sin(\pi\alpha)}\right). \tag{37}$$

The quantity $\chi$ lies in the interval $((1-\alpha)/2, 1-\alpha)$ (we assume $J\Delta > 0$, so that $\kappa = -1$). For $|\Delta| > |J|$, the winding number is ill-defined, and the Wiener-Hopf technique is not applicable.

To finish the discussion of the power-law models, we point out the following pattern: the long-range behavior of the MZM wave functions is determined by the character of the singularities of $Q(z)$ on the unit circle – in our case, at $z = 1$ (see Appendix A). These singularities, in turn, are determined by the asymptotic behaviors of $t_l$ and $\Delta_l$ in the limit of large $l$. Hence, the obtained asymptotic behaviors of $s_l$ are applicable not only for our particular model with pairing and hopping amplitudes given exactly by Eqs. (26) and (27), but for a much wider class of models, where the behavior of $t_l$ and $\Delta_l$ is described by Eqs. (26) and (27) in the limit $l \to \infty$.

### D. Exponential falloff of hopping amplitudes

In Ref. [26], the boundaries of the topological phases for the following model with short-range pairing and long-range hopping with exponential falloff with distance have been discussed:

$$t_l = \begin{cases} -\mu & \text{for } l = 0 \\ t_1 a^{|l|-1} & \text{for } l \ne 0 \end{cases}, \tag{38}$$

$$\Delta_l = \begin{cases} 0 & \text{for } l \ne \pm 1 \\ \Delta\mathrm{sgn}(l) & \text{for } l = \pm 1 \end{cases}, \tag{39}$$

where $0 < a < 1$. The function $Q(z)$ equals

$$Q(z) = \frac{t_1 z}{1-az} + \frac{t_1}{z-a} - \mu + \Delta(z - z^{-1}). \tag{40}$$

To determine its Cauchy index, the same considerations as in Appendix A can be used, which yield that the Cauchy index is given by the same equation as for the power-law model – see Eq. (30).

Let us consider the case $\kappa = -1$, when Eq. (3) has a nontrivial solution. The function $Q(z)$ is rational, so that the factors $Q_+(z)$ and $Q_-(z)$ can be found even without using Eqs. (13) and (14) if the poles and roots of $Q(z) = 0$ are known. The equation $Q(z) = 0$ is equivalent to a quartic equation, and its four roots can be calculated analytically if desired [29]. When $\kappa = -1$, three of these roots – $z_1$, $z_2$ and $z_3$ – lie outside the unit circle. These roots as well as the pole at $z = a^{-1}$ are contained in the factor $Q_+(z)$:

$$Q_+(z) = \frac{(z-z_1)(z-z_2)(z-z_3)}{1-az}. \tag{41}$$

The integral in Eq. (3) is determined by the residues at the three poles of $Q_+^{-1}(z)$:

$$s_l = -\sum_{n=1}^{3} \frac{1}{z_n^{l+1} Q'_+(z_n)}. \tag{42}$$

The asymptotic behavior of $s_l$ in the limit $l \to \infty$ is determined by the root (or roots) of $Q_+(z)$ with the smallest absolute value. Let us derive some properties of these roots. One of these roots is always negative, because $Q(-1)$ and $Q(-\infty)$ have different signs. The other two roots can be real or complex. In the limit of very large $|\Delta|$, an approximate solution of the equation $Q(z) = 0$ yields

$$z_1 \approx -1 - \frac{Q(-1)}{2\Delta}, \qquad z_2 \approx 1 - \frac{Q(1)}{2\Delta}, \tag{43}$$

$$z_3 \approx a^{-1} + \frac{t_1 a^{-1}}{\Delta(1-a^2)}. \tag{44}$$

In the opposite limit of small $|\Delta|$ we can obtain

$$z_1 \approx \frac{\mu + a^{-1} t_1}{\Delta}, \tag{45}$$

$$z_2 \approx z_2^{(0)} \left( 1 - \frac{\Delta \left| 1 - a z_2^{(0)} \right|^2}{t_1 + a\mu} \right), \qquad z_3 = z_2^*, \tag{46}$$

$$z_2^{(0)} = \frac{2t_1 a + (a^2+1)\mu + i(1-a^2)\sqrt{-Q(1)Q(-1)}}{2(t_1 + a\mu)}. \tag{47}$$

## V. ENERGY OF THE EDGE MODE IN A FINITE CHAIN

In this Section, we will obtain estimates for the energy of the edge states composed of two MZMs in finite chains. We will consider the Hamiltonian (1) with $l, n = 0..L$. For simplicity, we assume that the Cauchy index of $Q(z)$ equals $-1$. Then, there is one MZM corresponding to the left edge and one mode corresponding to the right edge of the chain (the described below approach can be easily generalized for the case of multiple MZMs per edge). Their wave functions are $(u_l, u_l)^T$ and $(u_{L-l}, -u_{L-l})^T$, respectively. The coefficient $u_l$ satisfy the equations

$$\sum_{n=0}^{\infty} (t_{l-n} + \Delta_{l-n}) u_n = 0, \quad l \geq 0. \tag{48}$$

The eigenfunction of the BdG Hamiltonian is a superposition of the two defined above wave functions with equal weights. The energy $E_0$ corresponding to this eigenfunction can be estimated as the matrix element of the BdG Hamiltonian between $(u_l, u_l)^T$ and $(u_{L-l}, -u_{L-l})^T$:

$$\begin{aligned} E_0 &\sim \textstyle\sum_{n,l=0}^{L} (u_{L-l}, -u_{L-l}) \begin{pmatrix} t_{l-n} & \Delta_{l-n} \\ \Delta^*_{n-l} & -t_{n-l} \end{pmatrix} \begin{pmatrix} u_n \\ u_n \end{pmatrix} \\ &= 2 \textstyle\sum_{n,l=0}^{L} u_{L-l} (t_{l-n} + \Delta_{l-n}) u_n. \end{aligned} \tag{49}$$

For further transformations we use Eq. (48):

$$E_0 \sim -2 \sum_{l=-\infty}^{-1} \sum_{n=0}^{L} u_{L-l} (t_{l-n} + \Delta_{l-n}) u_n. \tag{50}$$

To obtain an order of magnitude estimate for $E_0$, we need to know the coefficients $u_l$ with appropriate normalization, which we did not calculate. However, to determine the asymptotic behavior of $E_0$ in the limit of large $L$, we need to know only the behavior of $u_l$ in the limit of large $l$.

First, let us consider the case when the MZM wave function falls off exponentially fast in the limit of large $l$: $u_l \propto e^{-bl}$, $b > 0$. We have then

$$\begin{aligned} E_0 &\propto \sum_{l=-\infty}^{-1} \sum_{n=0}^{L} e^{bl - bL} (t_{l-n} + \Delta_{l-n}) u_n \\ &\approx e^{-bL} \sum_{l=-\infty}^{-1} \sum_{n=0}^{\infty} e^{bl} (t_{l-n} + \Delta_{l-n}) u_n \propto e^{-bL}. \end{aligned} \tag{51}$$

The double series here is always convergent: the sum is proportional to $p(e^b)$ [see Eq. (8)].

Next, consider the case when $t_l$ and $\Delta_l$ are given by Eqs. (26) and (27), respectively, and $\delta \equiv \min(\alpha, \beta) > 1$. Then, the asymptotic behavior of the MZM wave functions is given by Eq. (33). We have then in the limit of large $l$

$$\begin{aligned} E_0 &\propto \sum_{l=-\infty}^{-1} \sum_{n=0}^{L} \frac{1}{|L-l|^\delta} (t_{l-n} + \Delta_{l-n}) u_n \\ &\approx \frac{1}{L^\delta} \sum_{l=-\infty}^{-1} \sum_{n=0}^{\infty} (t_{l-n} + \Delta_{l-n}) u_n \propto L^{-\delta}. \end{aligned} \tag{52}$$

The series here is convergent as long as $\delta > 1$. Equation (52) is consistent with the numerical $E_0$ vs. $L$ dependence found in Ref. [18].

When $\delta < 1$ and $\alpha < \beta$, we have $E_0 \propto L^{-1}$, as demonstrated in Appendix B.

## VI. CONCLUSION

To sum up, using the Wiener-Hopf technique, we have developed a method to calculate analytically the wave functions of MZMs in semi-infinite Kitaev chains belonging to the BDI symmetry class. This method is applicable to chains with both finite-range and infinite-range couplings. The explicit analytical zero-energy solutions of the BdG equations illustrate the bulk-boundary correspondence principle: the number of MZMs equals the winding number of the Hamiltonian.

We have analyzed the asymptotic behaviors of MZM wave functions at large distances $l$ from the chain edge for several model Kitaev chains discussed in the literature. In particular, we proved analytically that in the case of exponential falloff of pairing and hopping amplitudes the MZM wave functions also fall off exponentially fast. In the case of power-law falloff of coupling amplitudes, $t_n \propto |n|^{-\alpha}$, $\Delta_n \propto |n|^{-\beta}$, with $\alpha > 1$ and $\beta > 1$, the wave functions fall off as $l^{-\delta}$ with $\delta = \min(\alpha, \beta)$. For $\beta < 1$ and $\beta < \alpha$, the winding number is ill-defined (this was described as a "half-integer winding number" in the literature), and massive Dirac edge states appear instead of MZMs. For $\alpha < \beta$ and $\alpha < 1$, the MZM wave function falls off as $l^{(\alpha-3)/2}$. For $\alpha = \beta < 1$, the wave function may exhibit a power-law falloff with a more complicated exponent.

We also studied the behavior of the energy $E_0$ of the fermionic edge mode composed of two MZMs in finite Kitaev chains with length $L$. More specifically, we have analyzed the asymptotic behavior of $E_0$ in the limit of large $L$. We found that $E_0 \propto e^{-bL}$, if the MZM wave function falls off as $e^{-bl}$ ($b > 0$) in the limit of large $l$ (even if $\Delta_l$ and $t_l$ exhibit power-law behavior). Within the model with power-law falloff of $t_l$ and $\Delta_l$, we found that $E_0 \propto L^{-\delta}$ for $\delta > 1$ (unless $\alpha = \beta$ and $J = \Delta$ in Eqs. (26) and (27), so that $E_0$ falls off exponentially fast), and $E_0 \propto L^{-1}$ for $\delta < 1$ and $\alpha < \beta$.

The obtained results are relevant for the description of Majorana modes in magnetic atom chains on superconductors (which can be studied using scanning tunneling microscopy) and in chains of cold atoms in optical lattices.

## ACKNOWLEDGMENTS

The author is grateful to A.S. Mel'nikov for useful comments on the paper. The work has been supported by Russian Science Foundation grant No. 21-12-00409.

## Appendix A: Analysis of the model with power-law falloff of pairing and hopping amplitudes

This appendix contains some technical details related to the analysis of MZM wave functions within the power-law model defined by Eqs. (26) and (27).

First, we will determine the value of the Cauchy index of the function $Q(z)$ given by Eq. (28). We will use the integral representation of the polylogarithm [30]:

$$\mathrm{Li}_\gamma(z) = \frac{z}{\Gamma(\gamma)} \int_0^\infty \frac{x^{\gamma-1}dx}{e^x - z}, \tag{A1}$$

where $\Gamma(\gamma)$ is the gamma function. For the imaginary part of $Q(z)$ on the unit circle we obtain

$$\begin{aligned} \mathrm{Im}[Q(e^{i\varphi})] &= 2\Delta \mathrm{Im}[\mathrm{Li}_\beta(e^{i\varphi})] \\ &= \frac{2\Delta \sin\varphi}{\Gamma(\beta)} \int_0^\infty \frac{e^x x^{\beta-1}dx}{|e^x - e^{i\varphi}|^2}. \end{aligned} \tag{A2}$$

The right-hand side here is non-zero for $\phi \neq 0$ and $\phi \neq \pi$, which indicates that the bulk spectrum of the chain is gapped, unless $Q(1) = 0$ or $Q(-1) = 0$. It also follows from this that the modulus of the winding number $\kappa$ can not exceed unity, so that $\kappa$ takes the values -1, 0 or 1. In the general case, when $Q(1)Q(-1) > 1$ the Cauchy index is even because $Q(z^*) = [Q(z)]^*$, and hence $\kappa = 0$ within our power-law model. The Cauchy index is odd when $Q(1)Q(-1) < 1$, and its sign coincides with the sign of $Q(1)\Delta$.

Now we will determine the asymptotic behavior of $s_l$ in the limit of large $l$ when either $\alpha \neq \beta$, or $\Delta \neq J$. Then, outside the unit circle $Q(z)$ has branch points at $z = 1$ and $z = \infty$, which should be connected by a branch cut. In Eq. (19) we can integrate along the contour $\ell$ shown in Fig. 1 instead of the unit circle. Such transformation is allowed if $Q(z)$ has no zeros between the unit circle and the contour $\ell$. This contour consists of two segments: $\ell_1$ goes along the circle $|z| = r$, and $\ell_2$ encloses the branch cut. Correspondingly, we can break down $s_l$ into two terms:

$$s_l = s_l^{(1)} + s_l^{(2)}, \tag{A3}$$

where

$$s_l^{(1)} = \frac{1}{2\pi i} \int_{\ell_1} \frac{dz}{Q_+(z) z^{l+1}} = \frac{1}{2\pi r^l} \int_0^{2\pi} \frac{e^{-il\beta} d\beta}{Q_+(re^{il\beta})}, \tag{A4}$$

$$s_l^{(2)} = \frac{1}{2\pi i} \int_{\ell_2} \frac{dz}{Q_+(z) z^{l+1}}. \tag{A5}$$

The integral in the right-hand side of Eq. (A4) is bounded, hence, $s_l^{(1)}$ is exponentially small in the limit of large $l$.

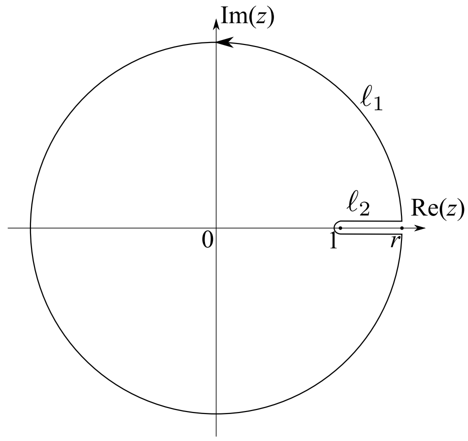


Figure 1. Deformed integration contour $\ell$.

To transform $s_l^{(2)}$, we substitute $Q_+(z) = Q(z)Q_-^{-1}(z)z$ into Eq. (A5) and switch to the integration variable $t = l \ln z$:

$$s_l^{(2)} = \frac{1}{2\pi i l} \int_0^{l \ln r} \frac{Q_-(e^{t/l})}{e^t} \left[ \frac{1}{Q(e^{t/l+i0})} - \frac{1}{Q(e^{t/l-i0})} \right] dt. \tag{A6}$$

To determine $Q(z)$ on both sides of the branch cut, we use the relation

$$\mathrm{Li}_\gamma(e^y) = \Gamma(1-\gamma)(-y)^{\gamma-1} + \sum_{n=0}^{\infty} \zeta(\gamma - n)\frac{y^n}{n!}, \tag{A7}$$

which is applicable for $|y| < 2\pi$ and for non-integer $\gamma$ [30]. We have then

$$\mathrm{Li}_\gamma(e^{y+i0}) - \mathrm{Li}_\gamma(e^{y-i0}) = \frac{2\pi i}{\Gamma(\gamma)} y^{\gamma-1} \tag{A8}$$

for $y > 0$, and

$$Q(e^{y+i0}) - Q(e^{y-i0}) = \frac{2\pi i \Delta}{\Gamma(\beta)} y^{\beta-1} - \frac{2\pi i J}{\Gamma(\alpha)} y^{\alpha-1}. \tag{A9}$$

In the limit of large $l$ we transform $s_l^{(2)}$ as follows:

$$\begin{aligned} s_l^{(2)} &= \int_0^{l \ln r} \frac{e^{-t} Q_-(e^{t/l})}{|Q(e^{t/l+i0})|^2} \left[\frac{\Delta}{\Gamma(\beta)} \frac{t^{\beta-1}}{l^\beta} - \frac{J}{\Gamma(\alpha)} \frac{t^{\alpha-1}}{l^\alpha}\right] dt \\ &\approx \frac{Q_-(1)}{Q(1)^2} \int_0^\infty \left[\frac{\Delta}{\Gamma(\beta)} \frac{t^{\beta-1}}{l^\beta} - \frac{J}{\Gamma(\alpha)} \frac{t^{\alpha-1}}{l^\alpha}\right] e^{-t} dt = \frac{Q_-(1)}{Q(1)^2} \left[\frac{\Delta}{l^\beta} - \frac{J}{l^\alpha}\right]. \end{aligned} \tag{A10}$$

Similar calculations can be performed in the case $\alpha < 1$, $\alpha < \beta$. First, we determine $Q_+(z)$ for $z$ close to 1 by integrating in Eq. (13) along the deformed contour shown in Fig. 1:

$$\frac{Q_+(z)}{Q_1(z)} = \exp\left(\frac{1}{2\pi i} \int_1^r \frac{\ln Q(t+i0) - \ln Q(t-i0)}{t-z} dt\right), \tag{A11}$$

$$Q_1(z) = \exp\left(\frac{1}{2\pi i} \int_{\ell_1} \frac{\ln(Q(t) t^{-\kappa})}{t-z} dt\right). \tag{A12}$$

The logarithm in Eq. (A11) should be continuous on the contour $\ell_2$ (for $\eta_+ > 0$). Using Eqs. (28) and (A7), on the real axis for $z > 1$ and in the vicinity of $z = 1$ in the leading order we obtain

$$Q(z \pm i0) \approx -2J\Gamma(1-\alpha) \sin\left(\frac{\pi\alpha}{2}\right) e^{\pm i\pi(1-\alpha)/2} (z-1)^{\alpha-1}. \tag{A13}$$

Substituting this into Eq. (A11) we find that

$$\begin{aligned} Q_+(z) &\approx Q_1(z) \exp\left(\frac{1-\alpha}{2} \int_1^R \frac{dt}{t-z}\right) \\ &= \tilde{Q}_1(z)(1-z)^{(\alpha-1)/2}, \end{aligned} \tag{A14}$$

where $\tilde{Q}_1$ is approximately constant in the vicinity of $z = 1$. Next, we substitute Eq. (A14) into Eq. (19) assuming $\kappa = -1$. Again, we integrate along the deformed contour shown in Fig. 1 to obtain in the limit of large $l$ (see similar calculations above)

$$\begin{aligned} s_l &\approx \frac{1}{2\pi i} \int_{\ell_2} \frac{dz}{Q_+(z) z^{l+1}} \approx -\frac{\tilde{Q}_1^{-1}(1)}{\pi} \cos\left(\frac{\pi\alpha}{2}\right) \int_1^R \frac{dz}{z^{l+1}} (z-1)^{\frac{1-\alpha}{2}} \approx -\frac{\tilde{Q}_1^{-1}(1)}{\pi l} \cos\left(\frac{\pi\alpha}{2}\right) \int_0^\infty e^{-t} (e^{t/l} - 1)^{\frac{1-\alpha}{2}} dt \\ &\approx -\frac{\tilde{Q}_1^{-1}(1)}{\pi l} \cos\left(\frac{\pi\alpha}{2}\right) \int_0^\infty e^{-t} \left(\frac{t}{l}\right)^{\frac{1-\alpha}{2}} dt = -\frac{\tilde{Q}_1^{-1}(1)}{\pi l^{\frac{3-\alpha}{2}}} \cos\left(\frac{\pi\alpha}{2}\right) \Gamma\left(\frac{3-\alpha}{2}\right). \end{aligned} \tag{A15}$$

## Appendix B: Asymptotic behavior of the energy $E_0$ within the power-law model with $\alpha < 1$

In this appendix, we will determine the asymptotic behavior of the energy $E_0$ in the limit of large chain lengths $L$ within the model where $t_l$ and $\Delta_l$ are given by Eqs. (26) and (27), respectively, and additionally $\alpha < 1$, $\alpha < \beta$. We also assume that $\kappa = -1$. For a start, we transform Eq. (50):

$$E_0 \sim S_1 + S_2, \tag{B1}$$

$$S_1 = -2 \sum_{l=-\infty}^{-1} \sum_{n=0}^{\infty} u_{L-l} (t_{l-n} + \Delta_{l-n}) u_n, \tag{B2}$$

$$S_2 = 2 \sum_{l=-\infty}^{-1} \sum_{n=L+1}^{\infty} u_{L-l}(t_{l-n} + \Delta_{l-n}) u_n. \quad \text{(B3)}$$

It is relatively easy to determine the asymptotic behavior of $S_2$:

$$\begin{aligned} S_2 &\propto \sum_{l=-\infty}^{-1} \sum_{n=L+1}^{\infty} \frac{1}{(L-l)^{\frac{3-\alpha}{2}} (l-n)^{\alpha} n^{\frac{3-\alpha}{2}}} \\ &\approx \int_{-\infty}^{0} dl \int_{L}^{\infty} dn \frac{1}{(L-l)^{\frac{3-\alpha}{2}} (l-n)^{\alpha} n^{\frac{3-\alpha}{2}}} \\ &= \frac{1}{L} \int_{-\infty}^{0} dl \int_{1}^{\infty} dn \frac{1}{(1-l)^{\frac{3-\alpha}{2}} (l-n)^{\alpha} n^{\frac{3-\alpha}{2}}} \propto \frac{1}{L}. \end{aligned} \quad \text{(B4)}$$

To estimate $S_1$, we use that fact that $u_n = s_n/2$:

$$S_1 = -\frac{1}{2} \sum_{l=-\infty}^{-1} s_{L-l} p_l, \quad \text{(B5)}$$

where the coefficients $p_l$ are introduced in Eq. (9). The sum in Eq. (B5) equals an expansion coefficient in the Laurent series of $s(z)p(z)$, so that

$$S_1 = -\frac{1}{4\pi i} \oint_{|z|=1} \frac{p(z)s(z)dz}{z^{L+1}}. \quad \text{(B6)}$$

From Eq. (15) we find that $s(z) = Q_+^{-1}(z)$, $p(z) = Q_-(z)/z$ up to a normalization factor, which does not depend on $L$. Taking into account Eq. (11), we obtain

$$S_1 \propto \frac{1}{4\pi i} \oint_{|z|=1} \frac{Q(z)dz}{Q_+^2(z) z^{L+1}}. \quad \text{(B7)}$$

Further calculations are made in the same spirit as the calculations of $s_l$ in Appendix A. We integrate along the deformed contour shown in Fig. 1 and neglect the exponentially small contribution from the segment $\ell_1$. Using Eqs. (A13) and (A14), we obtain

$$\begin{aligned} S_1 &\propto \frac{1}{4\pi i} \int_1^r \frac{dz}{z^{L+1}} \left[ \frac{Q(z+i0)}{Q_+^2(z+i0)} - \frac{Q(z-i0)}{Q_+^2(z-i0)} \right] \\ &\propto \int_1^r \frac{dz}{z^{L+1}} \propto \frac{1}{L}. \end{aligned} \quad \text{(B8)}$$

Both components of $E_0$ – $S_1$ and $S_2$ – are proportional to $L^{-1}$. Strictly speaking, these contributions can cancel each other out, however, numerical diagonalizations of the BdG Hamiltonians of finite chains performed by the author demonstrate that this does not happen, and the energy $E_0$ is proportional to $L^{-1}$.


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