Linear and non-linear transport across a finite Kitaev chain: an exact analytical study

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We present exact analytical results for the differential conductance of a finite Kitaev chain in an N-S-N configuration, where the topological superconductor is contacted on both sides with normal leads. Our results are obtained with the Keldysh non-equilibrium Green’s functions technique, using the full spectrum of the Kitaev chain without resorting to minimal models. A closed formula for the linear conductance is given, and the analytical procedure to obtain the differential conductance for the transport mediated by higher excitations is described. The linear conductance attains the maximum value of $e^2/h$ only for the exact zero energy states. Also the differential conductance exhibits a complex pattern created by numerous crossings and anticrossings in the excitation spectrum. We reveal the crossings to be protected by the inversion symmetry, while the anticrossings result from a pairing-induced hybridization of particle-like and hole-like solutions with the same inversion character. Our comprehensive treatment of the Kitaev chain allows us also to identify the contributions of both local and non-local transmission processes to transport at arbitrary bias voltage. Local Andreev reflection processes dominate the transport within the bulk gap and diminish for higher excited states, but reemerge when the bias voltage probes the avoided crossings. The non-local direct transmission is enhanced above the bulk gap, but contributes also to the transport mediated by the topological states.

I. INTRODUCTION

The search for Majorana zero modes (MZM) in topological superconductor systems is currently an intensely pursued quest in condensed matter physics,1–4 with the primary aim to realize a robust framework for topological quantum computing.5–7 Currently the most advanced experimentally platform for Majorana devices are based on proximitized semiconducting nanowires,8–10 although they have not yet been unambiguously proven to host Majorana states. Transport properties of Majorana nanowire devices have been intensively studied, with the main purpose of devising a detection scheme for the Majorana states by determining their transport fingerprints. The most fundamental one, that of observing a quantized zero bias peak in conductance, can be mimicked by trivial Andreev bound states,11,12 or level repulsion in multiband systems,13,14 thus several detection schemes exploiting also Majorana non-locality have been proposed.15–20 From the point of view of the applications, one of the schemes for the readout of Majorana qubits is based on transport interferometry,21,22 providing further motivation to explore the transport properties of Majorana devices.

Most of the works in this domain are out of necessity either numerical or based upon a minimal model, concentrating on charge transport through the in-gap states.10,11,13,22,23 Our aim is to find an analytical expression for the current flowing through a topological superconductor, taking into account its full excitation spectrum. The knowledge of such analytical solutions for at least one topological superconductor is instrumental in testing the reliability of the numerical results. As our model system we take a prototypical topological superconductor, the Kitaev chain.24 Although the low energy spectrum of a Kitaev chain with two Majorana states has served as the basis for the minimal models of nanowire transport, we are aware of only few analytical studies which focused on the transport characteristics of the Kitaev chain itself, achieving its description in analytical terms for several parameter ranges.24–29 Doorenbal et al.28 treat the chain as a fragment of an N-S-N system, but with the bias drop occurring at one contact only, which yields the well known value $2e^2/h$ for the conductance through an MZM. Without a self-consistent calculation it leads however also to non-conservation of current.29 Another recent work30 studied the transport properties of a Kitaev chain with long-range superconducting pairing, using a Green’s functions technique combined with the scattering matrix approach. The transport calculation is analytical, although it needs as input the eigenvectors, which are obtained from a numerical diagonalization of the Hamiltonian. Moreover, the authors focus only on the low-energy transport.

In this work we use the Keldysh non-equilibrium Green’s functions technique (NEGF) and derive analytical expressions for both the current and conductance of a Kitaev chain in an N-S-N configuration, in the linear as well as non-linear transport regime, for arbitrary hopping $t$, superconducting pairing $\Delta$ and chemical potential $\mu$. Thus we can access not only the known transport properties of the topological states, but also of the higher excited states.

While we derive the differential conductance for arbitrary bias drop at the contacts, we show only the results for symmetric bias – the configuration in which the current is conserved. In consequence, the crossed Andreev reflection processes do not contribute to transport. For the chosen symmetric setup, the transport occurs via two mechanisms, local Andreev reflection and non-local direct transmission. Both contributions feature conductance peaks resonant with the excitation energies, but
with different weights. The transport within the bulk gap is dominated by the local, Andreev processes, while the main contribution to transport above the bulk gap comes from the non-local, direct transmission processes. The excitation spectrum above the bulk gap contains several series of crossings and avoided crossings, ubiquitous in the spectra of Majorana nanowires, but to our knowledge not yet explained. We find that the crossings are protected by the inversion symmetry of the normal chain – the degenerate eigenstates have particle (hole) sectors of opposite inversion character. On the other hand, the particle (hole) sectors of anti-crossing states match under inversion, and the superconducting pairing allows the particle-like and hole-like solutions of the linear chain to hybridize. Inside the anticrossings the Andreev reflection processes are revived, reminiscent of their importance in the subgap transport. Similarly, even though the direct transmission plays the prominent role in the high bias conductance, it is also responsible for some of the current flowing through the two topological states at low bias. We obtain the maximum value of $e^2/h$ for the zero bias Majorana conductance peak, as expected from an NSN setup with symmetric bias drop. Remarkably, our results show that for a finite chain the value $e^2/h$ for the linear conductance is not obtained in the whole topological phase, but only near the “Kitaev points” ($\mu = 0$, $|t| = |\Delta|$). Elsewhere the conductance can be close to its maximum value or even significantly lower. We emphasize again that our results are the first complete analytical treatment of transport across a Kitaev chain, which provides a valuable benchmark for the numerical calculations, also of other model systems for 1D topological superconductors.

This paper is organized as follows. First, we analyze the spectrum of an isolated Kitaev chain in Sec. II including the higher excitations. In Sec. III we discuss our N-S-N transport setup, providing a general current formula for our system. The analytical expression for the linear conductance is derived in Sec. IV In Sec. V we present the formula for the differential conductance at finite bias in terms of appropriate Green’s functions. The detailed derivations of the expressions for the current, conductance and the Green’s functions are given in the Appendices.

II. THE ISOLATED KITAEV CHAIN

The central element of our N-S-N system is the finite Kitaev chain, which is a tight-binding chain of $N$ lattice sites, with one spinless fermionic orbital at each site and nearest-neighbor $p$-wave superconducting pairing. The $p$-wave nature of the superconductivity couples particles of equal spin, allowing a spinless treatment. The pairing is treated in the usual mean-field approach, yielding the Kitaev grandcanonical Hamiltonian

\[ \hat{H}_{KC} := \hat{H}_0 - \mu \hat{N}_{KC} = -t \sum_{j=1}^{N-1} (d_j^\dagger d_{j+1} + d_{j+1}^\dagger d_j) + \Delta \sum_{j=1}^{N-1} (d_j^\dagger d_{j+1} + d_{j+1}^\dagger d_j) - \mu \sum_{j=1}^{N} d_j^\dagger d_j, \]

in terms of the fermionic creation (annihilation) operators $d_j^\dagger$ ($d_j$). The quantities introduced in Eq. (1) are the real space position index $j = 1, \ldots, N$, the hopping amplitude $t \in \mathbb{R}$ and the superconducting pairing constant $\Delta \in \mathbb{R}$. The action of the gate voltage applied later to the wire is to change the chemical potential as $\mu \to \mu + \mu_g$, with $\mu_g = \eta g eV_g$, and $\eta_g$ the lever arm of the junction.

The spectrum and topological properties of both finite and infinite Kitaev model were discussed in detail in the recent past, and we shall give here only a brief overview of the low energy spectrum, giving more emphasis to the hitherto unexplored quasiparticle states at higher energy.

In the thermodynamic limit ($N \to \infty$) the energy of the excitations obeys the bulk dispersion relation

\[ E_{\pm}(k) = \pm \sqrt{[\mu + 2t \cos(kd)]^2 + 4\Delta^2 \sin^2(kd),} \]

where $d$ is the lattice constant. The topological features of the Kitaev chain can be found after a calculation of the winding number or the Pfaffian topological invariant. The boundaries between trivial and non-trivial phases in the topological phase diagram are determined by the gap closing of the bulk dispersion relation, which happens at $k = 0$ or $k = \pi/d$ for $\Delta \neq 0$ and $\mu = \pm 2t$. As one finds, the non trivial phase exists only for $|\mu|/\Delta < 2|t|/\Delta$.

In a finite chain, the bulk-edge correspondence implies the existence of evanescent state solutions at the system’s boundary in the topologically non-trivial phase. These states have a complex wavevector $k$, and their wave functions decay away from the edges with a decay length $\xi$, which for $\mu = 0$ is given by

\[ \xi = \frac{2d}{\ln \left| \frac{t-\Delta}{t+\Delta} \right|}. \]

The energy of these topological excitations lies inside the bulk gap introduced with Eq. (2) and is in general non-zero, with the upper bound proportional to $\exp(-N\xi)$; i.e. for $\xi \ll Nd$ the edge state energy is exponentially small. The energy of the decaying states becomes exactly zero for specific parameter settings, namely

\[ \mu_n = 2\sqrt{t^2 - \Delta^2} \cos \left( \frac{n\pi}{N+1} \right), \]

with $n = 1, \ldots, N$ and for $t^2 \geq \Delta^2$. Zero energy solutions for $t^2 < \Delta^2$ are found only for $n = (N+1)/2,$
which is only possible for odd $N$. The zero energy solutions form lines in the $(t/\Delta, \mu/\Delta)$ plane (we shall call them Majorana lines) departing from the points $|t| = |\Delta|$, $\mu = 0$, as depicted in Fig. 1.

The exact zero energy solutions of the isolated Kitaev chain represent fermion parity switches and for given $t, \Delta$ occur for discrete values of $\mu$. Close to the Majorana lines one always finds eigenstates with exponentially small energy, as seen in Fig. 1. Thus, due to the broadening of the energy levels induced by the coupling to the leads, also states with energy smaller than such broadening will effectively act as MZM. As we shall show, in an N-S-N setup with symmetric bias they yield a linear conductance very close to $e^2/h$, reaching the exact $e^2/h$ in the thermodynamic limit \cite{24,34,52,54}.

We recall here that in an N-S configuration the height of the zero bias peak is expected to be $2e^2/h$ \cite{110}. \footnotemark[10]

\begin{figure}[htb]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Ground state energy of the isolated Kitaev chain as a function of $t/\Delta$ and $\mu/\Delta$. The color map in the background displays the numerically calculated energy of the lowest eigenstate, the red line depicts the phase boundary $|\mu| = 2|t|$ between the topologically trivial ($|\mu| > 2|t|$) and non-trivial ($|\mu| < 2|t|$) bulk phases, while the white dashed lines are the “Majorana lines” defined by Eq. (4). Along these lines the ground state energy $E_0$ is exactly zero. All Majorana lines start from the $\mu = 0, t = \pm \Delta$ points and are located in the topological bulk region.}
\end{figure}

A. Higher excitation spectrum

The low energy states of the topological superconductors have garnered so far the most attention of the scientific community. Nevertheless, a current flowing through the Kitaev chain at a larger bias will involve also the higher lying excitations. Thus some questions naturally arise, such as: how will the high energy spectrum impact the differential conductance? If a chain is in the topological phase, will this affect the features visible at finite bias? To answer these questions we first analyze the full spectrum of a finite Kitaev chain. The numerically obtained spectrum as a function of $\mu$ is shown in Fig. 2(a) for $t > \Delta$, and in Fig. 2(b) for $\Delta > t$. The eigenstates in the Bogoliubov – de Gennes representation are composed of particle ($u$) and hole ($v$) components. In most of the spectrum the eigenstates have either particle ($|u| > |v|$) or hole ($|v| > |u|$) character; the states within the bulk gap (cf. Appendix A) but also some higher energy solutions described below, are nearly equal mixtures of both.

The linear chain, which is the foundation of the Kitaev chain in Eq. (1), has inversion symmetry. This property is also present in the superconducting system, albeit in a less simple form (cf. Appendix C) – the particle and hole sectors in each eigenstate of the Kitaev chain must have opposite character under inversion symmetry (cf. Fig. 3 for a detailed discussion see Appendix C).

For $t > \Delta$ we see a series of anticrossings between the higher excitations, which occur throughout the spectrum. The particle-like and hole-like solutions of the normal chain in the Nambu space at the anticrossings have the same character under inversion, thus they can hybridize under the influence of the superconducting pairing. In consequence, the particle and hole sectors of the hybridized quasiparticle eigenstates have nearly equal weight. The crossings, on the other hand, are protected by the different inversion symmetries of the involved eigenstates, and have predominantly particle- or hole-like character. For $\Delta > t$ the character of the excitation spectrum is naturally different - higher absolute value of $\mu$ again separates the spectrum into particle- and hole-like sets of states, but at $\mu = 0$ the particle-hole mixing occurs within the whole spectrum. Unlike in the $t > \Delta$ case, both the strict and avoided crossings occur now also outside of the topological phase.

In order to pinpoint the positions of degenerate energies in the spectrum we have to revisit the general quantization rule for the wave vectors of the finite Kitaev chain. As we showed in Ref. \cite{39}, the eigenstates of the Kitaev chain require in general the knowledge of four wave numbers $\pm \kappa_{1,2}$ ($\kappa_1 \neq \pm \kappa_2$), since one has to satisfy two boundary conditions for electron and hole sectors separately. We use $\kappa_\Sigma := (\kappa_1 + \kappa_2)/2$, $\kappa_\Delta := (\kappa_1 - \kappa_2)/2$ for shortness. The values of $\kappa_{1,2}$ are indeed related and obey

\begin{equation}
\cos (\kappa_\Sigma) \cos (\kappa_\Delta) = -\frac{1}{2} \frac{\mu t}{t^2 - \Delta^2},
\end{equation}

which can be obtained from Eq. (2) by demanding $E(\kappa_1) = E(\kappa_2)$. Thus, Eq. (5) is in fact a bulk property of the system which also encodes the dependence of $\kappa_\Sigma, \kappa_\Delta$ on the chemical potential in a finite system. Together with the boundary conditions, it yields the quantisation rule of the finite Kitaev chain,

\begin{equation}
\frac{\sin^2 [\kappa_\Sigma (N + 1)]}{\sin^2 [\kappa_\Delta (N' + 1)]} = \frac{1 + (\frac{\Delta}{\Sigma})^2 \cot^2 (\kappa_\Delta)}{1 + (\frac{\Delta}{\Sigma})^2 \cot^2 (\kappa_\Sigma)}.
\end{equation}

The description in terms of $\kappa_{\Sigma,\Delta}$ compared with $\kappa_{1,2}$ is more convenient and one can rewrite the dispersion rela-
expression provides \( \cos \) and \((b) \quad \Delta = 4\). We focus first on zero energy crossings, before we turn to the excitations. We have

\[
E(\kappa) = E(\kappa) \quad \text{for all values of the parameters \( t, \Delta, \mu, N \).}
\]

At specific values of \( \mu \), where the inversion-protected degeneracies occur, \( \kappa_\Sigma \) and \( \kappa_\Delta \) obey additional constraints. We focus first on zero energy crossings, before we turn to the excitations. We have \( E(\kappa_\Sigma) = 0 \) for \( \cos^2(\kappa_\Sigma) = \mu^2 \). Applying Eq. (5) to the latter expression provides \( \cos^2(\kappa_\Delta) = t^2/(t^2 - \Delta^2) \) and thus ensures \( E(\kappa_\Delta) = 0 \). This constraint on \( \kappa_\Delta \) is equivalent to \( \cot^2(\kappa_\Delta) = 0 \), which in turn puts a restriction on the quantisation rule, namely \( \sin^2[\kappa_\Sigma (N + 1)] = 0 \), and leads to Eq. (8). The same conclusion can be reached if the first constraint is put on \( \kappa_\Delta \).

While a detailed derivation of the position of strict and avoided crossings for \( E \neq 0 \) can be found in the appendix C2, let us here summarize its results. The boundary conditions, together with the requirement of double degeneracy (higher degeneracies occur only for

\[
E^2(\kappa_\Sigma, \Delta) = \frac{1}{\cos^2(\kappa_\Sigma, \Delta)} \left[ 4(t^2 - \Delta^2) \cos^2(\kappa_\Sigma, \Delta) - \mu^2 \right] \times
\left[ \frac{t^2}{t^2 - \Delta^2} - \cos^2(\kappa_\Sigma, \Delta) \right],
\]

after the application of Eq. (5) on Eq. (2). Moreover, \( \kappa_\Sigma, \kappa_\Delta \) define the same state and \( E(\kappa_\Sigma) = E(\kappa_\Delta) \) for all values of the parameters \( t, \Delta, \mu, N \).

The special cases of either \( t = 0 \) or \( \Delta = 0 \) or \( t^2 = \Delta^2 \), constrain \( \kappa_\Sigma, \Delta \) to be selected zeros of \( \sin^2[\kappa_\Sigma, \Delta (N + 1)] \):

\[
\kappa_\Sigma = n \frac{\pi}{N + 1} \quad \text{or} \quad \frac{(N + 1 - n) \pi}{N + 1}, \quad n = 2, \ldots, N_{\text{max}}, \quad (8)
\]

\[
\kappa_\Delta = m \frac{\pi}{N + 1}, \quad m = 1, \ldots, n - 1, \quad (9)
\]

with \( N_{\text{max}} = N/2 \) (\( N_{\text{max}} = (N - 1)/2 \)) for even (odd) \( N > 3 \). These values indeed satisfy the boundary conditions since \( \sin^2[\kappa_\Sigma, \Delta (N + 1)] [1 + (\Delta/t)^2 \cot^2(\kappa_\Sigma, \Delta)] = 0 \), for both \( t \gg \Delta, \Delta \). For odd \( N \) we find additional \((N - 1)/2\) degeneracies at \( \mu = 0 \) corresponding to \((N - 1)/2\) allowed values for \( \kappa_\Delta \) if \( \kappa_\Sigma = \pi/2 \), for both \( E \geq 0 \). The

\[ \text{FIG. 2. Full spectrum of a Kitaev chain, for (a) } t = 4.1\Delta \quad \text{and (b) } \Delta = 4.1t. \quad \text{The color scale shows the particle/hole character of the corresponding eigenstate, expressed through } |u| - |v|, \text{ where } |u| \text{ and } |v| \text{ are the norms of the particle and hole parts of the eigenstate, respectively. The violet shaded regions show the bulk gap.} \]

\[ \text{FIG. 3. Inversion symmetry for chosen ranges of the full spectrum, for (a) } t = 4.1\Delta \quad \text{and (b) } \Delta = 4.1t. \quad \text{The color represents } I_u := |u|/|v|/|u|^2 \text{ for the particle sector and } I_v := |v|/|v|^2 \text{ for the hole sector \& light red for } u/v \text{ even under inversion } (I_{u/v} = +1), \text{ blue for } u/v \text{ odd under inversion } (I_{u/v} = -1). \text{ Thickness of the lines is proportional to } |u| \text{ and } |v| \text{ in the corresponding panel, and the dark dashed and dot-dot-dashed lines follow } E_u((2n + 1)\delta\kappa) \text{ and } E_v(2n \delta\kappa) \text{ from Eq. (2), respectively, with } \delta\kappa := \pi/(N + 1). \]
values of \( \mu \) where the crossings occur follow from the Eq. (5) for fixed values of \( t \) and \( \Delta \). While for both \( \Delta > t \) and \( \Delta < t \) the number of crossings is the same, their positions are not. The energy eigenvalues follow as usual from the dispersion relation in either Eq. (2) or Eq. (7).

The conditions for degenerate energy levels are illustrated in Fig. 3. The energies corresponding to \( \kappa_{1,2} = n_{1,2} \pi/(N+1) \) are shown with dashed and dot-dot-dashed lines for odd and even \( n_{1,2} \), respectively. The conditions (6), (8) are obeyed at the intersections of the lines with \( n_{1,2} \)ether both even or both odd, and indeed at these intersections we see strict crossings. On the other hand, the avoided crossing appear for \( n_{1,2} \) with different parities. In these cases \( \kappa_{\Sigma,\Delta} \) are not integer, but half-integer multiples of \( \pi/(N+1) \), and the quantization rule (6) implies

\[
1 + \left( \frac{\Delta}{t} \right)^2 \cot^2 \kappa_{\Sigma} = 1 + \left( \frac{\Delta}{t} \right)^2 \cot^2 \kappa_{\Delta},
\]

which can be fulfilled only if \( \Delta = 0 \) because \( \kappa_{\Delta} \neq \kappa_{\Sigma,\Delta} \mod \pi \). Hence, for \( \Delta \neq 0 \) these crossings are avoided. Interestingly, the values of \( E \) and \( \mu \) at their centers can be correctly calculated from Eqs. (2) and (5) by using \( \kappa_{\Sigma,\Delta} \) which are half-integer multiples of \( \pi/(N+1) \).

One can summarize that the \( E \neq 0 \) crossings and anticrossings follow the equidistant quantization of a linear chain, where \( \Delta = 0 \) in Eq. (1), but the specific values of \( \mu \) and the related energies depend on the non-zero \( \Delta \). Thus the higher excitation spectrum indeed bears signatures of the topological phase, since at the crossover into the topological phase two of the extended states localize, becoming the boundary modes. The energies and wave functions of the remaining extended states readjust to accommodate the presence of the topological states, although for the extended states this change is continuous.

### III. N-S-N TRANSPORT AND THE CURRENT FORMULA

In this section we introduce our transport setup, illustrated schematically in Fig. 4 and discuss the current formula. We place the Kitaev chain between two normal conducting leads, described by the grandcanonical Hamiltonians

\[
\hat{H}_\alpha - \mu \hat{N}_\alpha = \sum_k \epsilon_{k\alpha} \hat{c}_{k\alpha}^\dagger \hat{c}_{k\alpha}, \quad \alpha = L, R
\]

where \( \hat{c}_{k\alpha}^\dagger \) (\( \hat{c}_{k\alpha} \)) creates (destroys) a spinless fermion in state \( k \) and lead \( \alpha \). Note that \( \hat{H}_{KC} \) in Eq. (1) and \( \hat{H}_{\alpha} \) in Eq. (10) are written with the reference energy being the chemical potential \( \mu \) of the Kitaev chain. In the above description we consider leads in their eigenbasis.

Our N-S-N junction is completed with the tunneling Hamiltonian

\[
\hat{H}_T = \sum_k \left( t_L c_{kL}^\dagger d_1 + t_L d_1^\dagger c_{kL} \right) + \sum_k \left( t_R c_{kR}^\dagger d_N + t_R d_N^\dagger c_{kR} \right),
\]

which couples only the first (last) chain site to the contact \( L \) (\( R \)). We consider the tunneling elements \( t_{L,R} \) as \( k \)-dependent, real quantities. This setup is equivalent to a fully spin polarized system where the fixed spin \( \sigma \) is suppressed in the notation. The current through an N-S-N junction can be calculated with the NEGF approach.29,50 Since the Kitaev Hamiltonian in Eq. (1) is given in mean field, and thus breaks the conservation of particles, the calculation has to be carried out with care. The physical current measured in experiment is conserved everywhere, thus we calculate it for simplicity inside the left lead. There, the electronic current (for fixed spin) reads,

\[
I_L(t) = -e \langle \hat{N}_L \rangle,
\]

where \( e \) is the elementary charge and \( \hat{N}_L = \sum_k \hat{c}_{kL}^\dagger \hat{c}_{kL} \).

The steady state current (for fixed spin) reads

\[
I_L = \frac{e}{2h} \int dE \text{Tr} \left\{ \tau_z \otimes \mathbb{1}_N \Gamma_L \left[ G^\infty + F_L \left( G^r - G^a \right) \right] \right\},
\]

with \( \Gamma_\alpha = -2 \text{Im} (\Sigma_\alpha^\infty) \) (\( \alpha = L, R \)), where \( \Sigma_\alpha^\infty \) is the retarded self-energy of the lead \( \alpha \), defined in Appendix 4. Since we are working in the BdG formalism, all quantities under the trace in the above equation are \( 2N \times 2N \) matrices, defined w.r.t. \( \hat{\Psi} = \left( d_1, \ldots, d_N, d_1^\dagger, \ldots, d_N^\dagger \right)^T \), forming electronic and hole subspaces. For example, the matrix \( F_\alpha \) contains the Fermi functions \( f(E) \) for electrons and holes in the following form

\[
F_\alpha = \left[ \mathbb{1}_N f(E - eV_\alpha) \quad \mathbb{1}_N f(E + eV_\alpha) \right],
\]
where $V_L = \eta V$, $V_R = (\eta - 1)V$ account for scenarios with different applied bias $V$. Further, the lesser Green’s function $G^<$ is

$$G^< = iG^a \left( \sum_{\alpha=L,R} F_{\alpha} \Gamma_{\alpha} \right) G^a,$$  \hspace{1cm} (15)

with details of the derivation discussed in appendix [1].

In equilibrium ($V = 0$) we have $G^<_{\text{eq}} = -F(E) (G^+ - G^-)$ and the current vanishes.

The special choice of the tunneling Hamiltonian in Eq. [11] defines the self-energies $\Sigma_{\alpha}$ as sparse matrices, see Eqs. (E4), (E5). This, together with the trace and the particle-hole symmetry, yields a current formula where only two entries of the retarded Green’s function, namely $G^r_{1,N}$ and $G^r_{1,N+1}$, are required. One finds

$$I_L = \frac{e}{\hbar} \int_{R} dE \left\{ \Gamma_L \Gamma_R \left| G^r_{1,N} \right|^2 \left[ f(E - eV_L) - f(E - eV_R) \right] 
+ \Gamma_L \Gamma_R^+ \left| G^r_{1,N+1} \right|^2 \left[ f(E - eV_L) - f(E + eV_L) \right] \right\},$$  \hspace{1cm} (16)

now setting $V_L = -V_R = V/2$. We choose this scenario to keep the current in Eq. (16) conserved, $I_L = -I_R$, which for symmetric bias occurs if $\Gamma_L = \Gamma_R$, even without a self-consistent calculation of $\Delta$. The density of states in the lead $\alpha$ and the associated tunneling amplitudes $|t_{\alpha}(k)|^2$ are encoded in the quantities $\Gamma_{\alpha} = 2\pi \sum_{k} |t_{\alpha}(k)|^2 \delta(E \pm \epsilon_{k\alpha})$, with $- (+)$ for particles (holes). In a realistic device scenario one may have however to represent the leads in the site basis and employ a recursive approach to calculate the self-energies.

Eq. (16) allows a microscopic analysis of the charge transfer through the Kitaev chain, where two processes contribute. The term containing $G^r_{1,N}$ describes the usual direct transfer ($D$) of a quasiparticle from the left to the right lead through a normal conducting system, but here in presence of the p-wave superconductivity embodied by $\Delta$. The second term in Eq. (16), i.e. the one including $G^r_{1,N+1}$, describes the Andreev reflection – the incoming electron is reflected back as a hole and a right moving Cooper pair is formed inside the Kitaev chain. In the third possible process the right-moving Cooper pair in the chain is formed by an electron coming from the left and a hole coming from the right. This process, named crossed Andreev reflection, does not contribute to the current in a symmetric bias configuration. We give the exact analytic form of $G^r_{1,N}$ and $G^r_{1,N+1}$ in appendix [F].

The relative weight of the two contributing processes depends on the chosen parameters of the Kitaev chain ($\mu$, $t$, $\Delta$), as we will see in the context of the zero temperature conductance in the next section.

### IV. Linear Transport

The conductance $G := \lim_{V \to 0} \partial I / \partial V$ is easily calculated from Eq. (16). At $T = 0K$, one finds the simple formula

$$G = \frac{e^2}{h} \left\{ \Gamma_L \Gamma_R \left| G^r_{1,N} \right|^2 \left[ \Gamma_L \Gamma_R^+ \left| G^r_{1,N+1} \right|^2 \right] \right\}_{E=0} =: G_D + G_A,$$  \hspace{1cm} (17)

accounting for direct transport and Andreev reflection, respectively.

In the following we make use of the analytic expressions for $G^r_{1,N}$, $G^r_{1,N+1}$ derived in Appendix [F]. and for simplicity we consider the wide band limit, where the tunneling amplitudes $t_L$, $t_R$ and the densities of states $\rho_L$, $\rho_R$ in the leads are constant. Thus, $\Gamma_{L,R} = \Gamma_{L,R} = \text{const.}$ We find for the conductance the closed form

$$G = \frac{e^2}{h} \frac{\gamma_L \gamma_R (p^{N+1} + m^{N+1})^2}{|q_+|^2 + \gamma_L \gamma_R (p^{N+1} + m^{N+1})^2},$$  \hspace{1cm} (18)

with $p = t + \Delta$, $m = t - \Delta$ and $\gamma_{L,R} = \Gamma_{L,R}/2$. The polynomial $q_s$ ($s = \pm 1$), given by

$$q_s = p^{N-2} \left[ s p^2 x_{N,0} + i p x_{N-1,0} (s \gamma_L - \gamma_R) \right] + x_{N-2,0} \gamma_L \gamma_R,$$  \hspace{1cm} (19)

carries information on the spectral structure of the isolated Kitaev chain, since the determinant of the isolated Kitaev Hamiltonian with $N$ sites is $(-1)^N p^{2N} x_{N,0}$. The closed form of the term $x_{j,0}$ for an arbitrary integer $j$ is

$$x_{j,0} = \frac{R^j_{+1} - R^j_{-1}}{R_+ - R_-},$$  \hspace{1cm} (20)

with $R_{\pm} = (-\mu \pm \sqrt{\mu^2 - 4mp})/(2p)$.

The conductance in the limit $N \to \infty$ takes the value $e^2/h$. We also get the value $G = e^2/h$ for the linear conductance at the Kitaev points, independent of the value of the coupling strengths $\gamma_{L,R}$, since the terms in $q_s$ vanish there. The $G_L$ from equations (32),(33) in Ref. [28] can be obtained from our formula (18) by setting $\mu = 0$ and adding the factor 2 (in Ref. [28] one contact is effectively grounded).

Besides the Kitaev points the behavior of the conductance is more intricate and depends on the parameters setting. In particular, on the zero energy Majorana lines of the isolated chain, see Eq. (4), the term $x_{N,0}$ vanishes, although, due to the coupling to the leads, the whole polynomial $q_s$ does not. For the special case of symmetric coupling $\gamma_L = \gamma_R$ the conductance along the Majorana lines becomes however independent of the coupling. The behavior of the conductance in the $t/\Delta - \mu/\Delta$ plane is shown in Fig. [5](a,b) for the case of $N = 20$ and $N = 21$. While in the vicinity of the Kitaev points the conductance is large and close to $e^2/h$, as the ratio of $t/\Delta$ increases it remains so large only in close vicinity of the Majorana lines.
case, from the function $G_N(q)$, the difference between the Andreev and the direct term originates from the relation between in-gap states and $x_N$. In the region of the plateau $q_s$ is also small, thus $G_A$ is enhanced while $G_D$ is suppressed. In the limit of vanishing order parameter, $\Delta = 0$, it immediately follows from the above equations that $G = G_D$, $G_A = 0$, since as expected – the Andreev contribution vanishes. For $\xi \gg dN$ and leaving the discrete lines of non-zero conductance aside for a second, we find no in-gap states with zero, or even exponentially small energy anymore; the function $q_s$ grows for increasing values of $\mu/\Delta$ and/or $t/\Delta$, which leads to a suppression of both conduction terms $G_D \propto |q_-|^2/|q_+|^4$, $G_A \propto 1/|q_+|^4$. For intermediate parameter values $\xi \approx dN$, the polynomials $x_{N-1,0}, x_{N-2,0}$ become important. They describe essentially the spectrum of a Kitaev chain with $N - 1$, $N - 2$ sites, i.e. $\xi \gg d(N-j)$ for $j = 1, 2$. Their contributions define the crossover region between the triangular plateau of high conductance and the region featuring separated Majorana lines within the topologically non-trivial phase when $\xi \gg dN$. Note that the crossover region is influenced by $\gamma_{L,R}$ too.

Let us turn to the conductance along the Majorana lines, given by (4). On those lines the function $x_{N,0}$ vanishes and thus the functions $q_s$ have minima in $\mu$. The value of $q_s$ varies strongly around these minima and leads to the appearance of low conductance regions between the Majorana lines for $\xi \gg dN$. The ratio of $G_D$ and $G_A$ changes along those lines as depicted in Fig. 6 starting with $G_A = 1$ and $G_D = 0$ at Kitaev points and converges to $G_A = 0$ for $t/\Delta \rightarrow \infty$. This behavior is independent of the chosen line. Remarkably, the sum $G_D + G_A$ is seemingly constant and equal to $e^2/h$; it is in fact very slightly suppressed due to Eq. (18), becoming fully quantized only in the thermodynamic limit.

In order to better understand this behavior, we examine more closely the two contributions to the conductance, $G_D$ and $G_A$, see Eqs (17). We find

$$G_D = \frac{e^2}{h} \frac{\gamma_L \gamma_R \left(p^{N-1} + m^{N-1}\right)^2}{|q_+|^2 + \gamma_L \gamma_R \left(p^{N-1} + m^{N-1}\right)^2} |q_-|^2, \quad (21)$$

$$G_A = \frac{e^2}{h} \frac{\gamma_L^2 \gamma_R^2 \left(p^{2N-2} + m^{2N-2}\right)^2}{|q_+|^2 + \gamma_L \gamma_R \left(p^{N-1} + m^{N-1}\right)^2} |q_-|^2, \quad (22)$$

with $q_\pm$ from Eq. (19). For details of the calculation, see appendix [1]. The contributions $G_A$ and $G_D$ for the case $N = 20$ are depicted in Fig. 5(c), d). The difference between the Andreev and the direct term originates from the function $q_-$ which appears in the numerator of $G_D$. For $\gamma_{L,R} \ll \Delta$ the $q_-$ factor is small as long as $\xi \ll dN$, i.e. inside the triangular conductance plateau. Here $x_N$ is exponentially small due to the existence of in-gap states and $x_{N-1,0}, x_{N-2,0}$ are suppressed by $\gamma_{L,R}$. In the region of the plateau $q_s$ is also small, thus $G_A$ is enhanced while $G_D$ is suppressed. In the limit of vanishing order parameter, $\Delta = 0$, it immediately follows from the above equations that $G = G_D$, $G_A = 0$, since

FIG. 5. Conductance $G$ (wide band limit) in units of $e^2/h$ for $\gamma_{L,R}/\Delta = 0.001$ as function of $\mu/\Delta$ and $t/\Delta$. (a),(b) The roughly triangular plateau of high conductance is bounded (with some spreading) by the phase boundary (red line) and branches out into distinct lines when the magnitude of decay length and system length become comparable. Those lines of high conductance follow the Majorana lines given by Eq. (4), with one of them always coinciding with the $\mu = 0$ axis for odd $N$. (c) The most important contribution to the conductance $G = G_A + G_D$ is the Andreev term. (d) The direct term $G_D$ only broadens the conductance plateau.

FIG. 6. Conductance contributions $G_A$ and $G_D$ (wide band limit, $T = 0K$) in units of $e^2/h$ as function of $t/\Delta$ along the zero energy line, with $\mu$ adjusted to obey Eq. (4) for $n = 10$ and with $\gamma_L = \gamma_R = 0.001\Delta$ for different chain lengths. The Andreev term (solid lines) mostly contributes in the vicinity of the Kitaev point and decreases for larger ratios $t/\Delta$, while $G_D$ (dashed lines) shows the opposite behavior. The total conductance (black line) $G = G_A + G_D$ stays close to $e^2/h$, since a contributing zero energy eigenstate of the isolated Kitaev chain is always available. The Andreev term accounts here for the reflection $R_D = 1 - T_D$, where $T_D$ is the transmission amplitude of the direct term.
V. NON-LINEAR TRANSPORT

The non-linear transport effects are captured by the differential conductance $\partial I/\partial V$. At $T = 0$K and using Eq. (16) we find

$$\frac{\partial I}{\partial V} = \frac{e^2}{2h} \sum E = \pm V/2 \Gamma_L \left( \Gamma_R G_{1,N}^r |G_{1,N}|^2 + \Gamma_L G_{1,N+1}^r |G_{1,N+1}|^2 \right),$$

(23)

where we set $V_L = -V_R = V/2$. We depicted $\partial I/\partial V$ and its Andreev (A) and direct (D) contributions given by the $G_{1,N+1}^r$ terms in Figs. 7 and 8.

![Fig. 7. Differential conductance as a function of $eV/(2\Delta)$ and $\mu/\Delta$ for $|t/\Delta| = 4.1$, $\gamma_L = \gamma_R = 0.02\Delta$, and $N = 20$. (a) The Andreev term is the dominant contribution to the differential conductance for the in-gap states, but also affects the excitations. (b) The direct contribution to $\partial I/\partial V$ is present for all eigenstates, its strength inside the gap depends on the parameters. (c) The total differential conductance is the sum of the Andreev and direct terms. (d) The dark stripe for $V \approx 0$ of the Andreev term in (a) has in fact a braid-like structure, since the ratio of the decay length to the chain length, $\xi/dN$, is too large to support zero energy eigenstates everywhere. The Andreev reflections are stronger around the values of $\mu$ where exact zero energy states are present. Direct process contributions enhance the transport between two Andreev peaks.](image)

As expected, the Andreev term is slightly smaller than $e^2/h$ around $V \approx 0$ for $|\mu| < 2|t|$ and $\xi/(dN) \ll 1$, while the direct term is weak. Outside $V \approx 0$ the roles of Andreev and direct contributions are exchanged, though the Andreev term reemerges at the resonances with the quasiparticle energy levels and inside the avoided crossings between higher excitations; there the involved eigenstates of the Kitaev chain have again significant contributions from both particle and hole sectors (cf. Fig. 2). A special situation arises at the Kitaev points, where $\mu = 0$ and $|t| = |\Delta|$. Here the isolated Kitaev chain hosts only eigenstates with energies $0, \pm 2|t|$ (degenerate). For these parameters direct charge transfer through the Kitaev chain is forbidden. This becomes evident when the Kitaev chain Hamiltonian is represented in terms of Majorana operators (see Fig. 10), where one of the nearest neighbor hopping amplitudes, either $i(\Delta + t)$ or $i(\Delta - t)$, vanishes, and the chain falls apart into a set of dimers and two end sites. The direct term $G_{1,N}^r$ cannot contribute to transport, which occurs only through the Andreev term $G_{1,N+1}^r$ — as long as $\Gamma_R \neq 0$, the Cooper...
pair formed in the Kitaev chain through the Andreev reflection can escape into the right lead. When \( \mu \neq 0 \), the chemical potential binds Majorana operators of the same site and establishes a direct transport channel linking the dimers and end sites.

Let us turn back to the region around \( V \approx 0 \) for \( |\mu| < 2|t| \), \( \xi/(dN) \ll 1 \) and \( |\Delta| \neq |t| \). The seemingly structureless Andreev contribution to \( \partial V \) in Fig. 7(a) has in fact a braid-like pattern of larger values as depicted in panel (d) of Fig. 7. The higher values \( \approx \varepsilon^2/h \) for the Andreev term arise around the \( \mu \) values where the MZM are present \( ^{26,29} \), i.e. at the zero-energy crossings. In between these specific parameter values the importance of the Andreev contribution decreases and the direct term starts to contribute.

VI. CONCLUSIONS

In this work we have investigated linear and non-linear transport across a finite Kitaev chain in an N-S-N setup, with symmetrically applied bias. Using the analytical methods developed to study the spectrum of the isolated Kitaev chain \(^{29} \) we could provide closed formulas for the relevant Green's functions in turn for the linear and differential conductance at zero temperature. We have analyzed the quasiparticle spectrum with its complex pattern of strict and avoided crossings governed by the inversion symmetry, relating it to the calculated transport spectra. Our results show that direct transmission processes contribute to the subgap transport mediated by the topological states, and that the Andreev processes participate in the transport at high bias, especially when the involved states are nearly equal superpositions of particle and hole solutions. Further, remarkably, in a finite chain even along the Majorana lines the linear conductance is only approaching its maximum value of \( \varepsilon^2/h \), reaching it only near the Kitaev points.

In summary, our work provides a complete description of transport through an archetypal topological superconductor, extending our knowledge of this system beyond what can be gleaned from minimal models reduced to topological states alone.

ACKNOWLEDGMENTS

NL thanks for financial support the Elite Netzwerk Bayern via the IGK "Topological Insulators" and the Deutsche Forschungsgemeinschaft via SFB 1277 Project B04. BM would like to acknowledge funding from the Science and Engineering Research Board (SERB), Government of India under Grant No. STR/2019/000030, and the Ministry of Human Resource Development (MHRD), Grant no. STARS/APR2019/NS/226/FS under the STARS scheme.

APPENDIX A: BULK GAP

The bulk gap in the Kitaev spectrum is easily estimated from the dispersion relation (2). The condition for the vanishing first derivative at the band extrema is fulfilled at three values of bulk momentum \( k \),

\[
\begin{align*}
k_1 &= 0, & k_2 &= \pi, & k_0 &= \arccos \left( \frac{\mu t}{2(\Delta^2 - t^2)} \right).
\end{align*}
\]

Examples of the spectra of the Kitaev chain with \( N = 20 \) sites as a function of \( \mu \), together with the lines denoting the bulk energies at the band extrema, are shown in Fig. 9. The wave functions in a finite Kitaev chain can be described by purely real, purely imaginary or complex wave vectors \( \kappa \), in the regions marked in the figure. The bulk gap is marked with light red shading.

**FIG. 9.** The band extrema of a bulk Kitaev chain as a function of \( \mu \), for (a) \( t = 4.1|\Delta| \) and (b) \( \Delta = 4.1t \). The numerical energy levels for a chain with \( N = 20 \) sites are shown in grey for comparison. The types of allowed solutions for the wave number \( \kappa \) in a finite chain are indicated. Purely imaginary \( \kappa \) are allowed in the small range of \( \mu \) indicated in the inset of (a). The notation \( \kappa \in \mathbb{C} \) in the topological range of \( \mu \) in (b) means that the allowed wavevectors have also a constant real part, \( \pi/2 \).

APPENDIX B: SELECTED QUANTUM BASES FOR THE KITAEV CHAIN

The operators associated with the Kitaev chain can be represented in several bases, each suited to facilitate some specific calculation. We give here an overview of the four basis choices which will be used in these Appendices, together with the rationale behind this choice.

1. **Default Bogoliubov - de Gennes basis**, used throughout the main text and given by

\[
\Psi = (d_1, ..., d_N, d_1^\dagger, ..., d_N^\dagger)^T.
\]

This basis neatly separates particle and hole sectors of the system. The representations of the physical quantities in this basis do not carry any labels: the Green’s functions are \( G^s \), where \( s = <, >, a, r \), the self-energies \( \Sigma^s_\alpha \), the \( \Gamma \) matrices \( \Gamma_\alpha \).
2. Chiral basis is defined by
\[ \hat{\Psi}_c = (\gamma_1^A, \ldots, \gamma_N^A, \gamma_1^B, \ldots, \gamma_N^B)^T, \]  
where \( \gamma^{A/B} \) are the Majorana operators, given by 
\[ \gamma^A = \frac{(d_j + d_j^\dagger)}{\sqrt{2}}, \quad \gamma^B = \frac{i(d_j^\dagger - d_j)}{\sqrt{2}}. \]  
The Hamiltonian terms of the Kitaev chain in this basis are illustrated in Fig. 10. We name it “chiral” because in this basis the chiral symmetry has an especially simple representation, \( C = \sigma_z \otimes 1_{N \times N}. \) The physical quantities in this basis are denoted by the subscript \( c \), e.g. \( \tilde{\Psi} = (\Delta^\pm, \bar{\gamma}, \bar{\gamma}, \Delta^\mp)^T \).

3. Site-ordered particle-hole basis is just a rearranged default basis, with
\[ \hat{\Psi} = (d_1, d_1^\dagger, \ldots, d_N, d_N^\dagger)^T. \]
We denote the physical quantities in this basis by \( a^\dagger \), e.g. \( \tilde{G}^a, \tilde{\Sigma}_a \). The transformation between this and the default basis is given by \( \hat{\Psi} = U\hat{\Psi} \), with
\[
U_{nm} = \begin{cases} 
\delta_{m,(n+1)/2} & \text{for } n \text{ odd} \\
\delta_{m,2n+2} & \text{for } n \text{ even},
\end{cases}
\]
with \( n, m = 1, \ldots, 2N \). Since \( U \) is just a permutation matrix, an observable \( A \) transforms as \( \hat{A} = UAU^T \). This is our intermediate basis in Appendix D, in which the site-specific Green’s functions are expressed most conveniently.

4. Site-ordered Majorana basis is a rearranged chiral basis, with
\[ \hat{\Psi}_M = (\gamma_1^A, \gamma_1^B, \ldots, \gamma_N^A, \gamma_N^B). \]
The physical quantities in this basis are denoted by the subscript \( M \). The unitary transformation to the default basis, such that \( \hat{\Psi}_M = T\hat{\Psi} \), is given by the matrix \( T \)
\[
T = \frac{1}{\sqrt{2}} \begin{bmatrix}
1 & 0 & \cdots & 0 \\
-i & 0 & \cdots & 0 \\
0 & 1 & \cdots & 0 \\
0 & -i & \cdots & 0 \\
\end{bmatrix},
\]
where "|" separates the first \( N \) and the last \( N \) columns. The physical quantities transform as \( A_M = T A T^\dagger \). In the Appendix F, we take advantage of the tridiagonal form of the Hamiltonian in this basis (the elements of the Hamiltonian are illustrated in Fig. 10).

**Appendix C: Eigenvectors and degeneracies in the spectrum**

1. The general eigenvector problem and inversion symmetry

We briefly recapitulate here the eigenvalue problem investigated in Ref. [39] and introduce the inversion symmetry before we turn to the degenerate energy eigenvalues. The Kitaev chain Hamiltonian can be expressed in the chiral basis (cf. Eq. (B2)) through
\[ H_c = \begin{bmatrix} 0_{N \times N} & h \\ h^\dagger & 0_{N \times N} \end{bmatrix}, \]
with \( H_{KC} = \frac{1}{2} \hat{\Psi}_c^\dagger H_c \hat{\Psi}_c \) and \( h_{n,m} = -i\mu \delta_{n,m} + a \delta_{n,m+1} - b \delta_{n+1,m} \) for \( n, m = 1, \ldots, N \), \( a = i(\Delta - t) \), \( b = i(\Delta + t) \). For an eigenvector \( \vec{w} = (\vec{v}_A, \vec{v}_B)^T \) of the Hamiltonian \( H_c \) the sublattice vectors \( \vec{v}_A := (\xi_1, \ldots, \xi_N)^T \), \( \vec{v}_B := (\sigma_1, \ldots, \sigma_N)^T \) have to obey
\[ h \vec{v}_B = E \vec{v}_A, \quad h^\dagger \vec{v}_A = E \vec{v}_B. \]
In particular, we consider here exclusively the case of \( E \neq 0 \), where one can choose all \( \xi_n \) (\( \sigma_n \)) as real (pure imaginary) numbers. Solving for \( \vec{v} \) grants
\[ hh^\dagger \vec{v}_A = E^2 \vec{v}_A, \]
and \( \vec{v}_B \) follows then from Eq. (C3). Importantly, the entries of \( \vec{v}_A \) obey
\[ \xi_{j+2} = \frac{E^2 + a^2 + b^2 - \mu^2}{ab} \xi_j - \xi_{j-2} + i\mu (\frac{b-a}{ab} (\xi_{j-1} - \xi_{j+1}) \). \]
Extending the sequence of \( \xi \)'s via Eq. (C5) beyond the range \( j = 1, \ldots, N \) allows the simplification of the boundary condition to
\[ \xi_0 = \xi_{N+1} = b \xi_1 - a \xi_{-1} = b \xi_{N+2} - a \xi_N = 0, \]
while \( \vec{v}_A \) still contains only \( \xi_1, \ldots, \xi_N \) and the boundary condition yields after some algebra the quantisation rule given by Eq. (B3) given by Eq. (C6). A sequence obeying Eq. (C5)
requires four initial values, for example $\xi_{-2}$, $\xi_{-1}$, $\xi_0$, $\xi_1$, and one can derive the following closed formula

$$
\xi_j = \sum_{i=-2}^{1} \xi_i X_i(j),
$$

(C7)

where the functions $X_i(j)$, (cf. Eqs. (C27) - (G30) in the appendix [G2]) depend on $E^2$, $t$, $\Delta$, $\mu$ and $N$; they inherit the selective property $X_i(j) = \delta_{i,j}$ for only $i$, $j = -2 \ldots , 1$. As we see from the boundary conditions in Eq. (C7), $\xi_0 = 0$ and thus is fixed, while $\xi_{-1} = b \xi_j/a$. In the case of no degeneracy we have one degree of freedom and we can choose $\xi_1$ arbitrarily. Consequently, $\xi_{-2}$ is the last missing initial value and can be fixed via $\xi_{N+1} = 0$ yielding

$$
\xi_{-2} = -\xi_1 \left( a X_1(N+1) + b X_{-1}(N+1) \right) a X_{-2}(N+1)
$$

(C8)

in the absence of degeneracy. The eigenvector problem is now solved, since the constraint $b \xi_{N+2} - a \xi_N = 0$ quantizes the wave vectors generating the eigenvalue $E$ and thus the values of the functions $X_i(j)$ are known.

In our previous work we used a rather lengthy method to determine the entries of $\vec{v}_B$ from the ones of $\vec{v}_A$. The inversion symmetry $I$ allows us to pursue a much simpler method as we explain in the following. Upon inversion, i.e. $d_{ij}^{(t)} \rightarrow d_{N-i,j}^{(t)}$ in Eq. (1), one obtains back the Kitaev chain, but with $-\Delta$, due to the p-wave nature of the coupling. Thus, $I \hat{H}_{KC} I^{-1} = \hat{H}_{KC} |_{-\Delta}$ with $I$ being the operator of inversion symmetry in the BdG description. Written in the basis of $\mathcal{H}_c$, the representation of $I$ is

$$
I_c = \begin{bmatrix} I_0 & 1 \\ 1 & I_0 \end{bmatrix}, \quad I_0 = \begin{bmatrix} 1 \\ & \ddots \\ & & 1 \end{bmatrix},
$$

where $I_0$ represents the usual inversion operation, i.e. reversing the site order. The use of $I_c$ on the eigenvector problem yields

$$
(h|_{-\Delta}) I_0 \vec{v}_B = E I_0 \vec{v}_A, \quad (h^\dagger|_{-\Delta}) I_0 \vec{v}_A = E I_0 \vec{v}_B.
$$

Importantly, we have that $h|_{-\Delta} = -h^\dagger$ and vice versa, transforming the equations for $I_0 \vec{v}_A$ ($I_0 \vec{v}_B$) in the ones of $\vec{v}_B$ ($\vec{v}_A$) at $-E$. Recalling that all $\vec{v}_A$ ($\vec{v}_B$) are real (pure imaginary) vectors, we can cancel this sign of $E$ by the now obvious relation between $\vec{v}_A$ and $\vec{v}_B$

$$
\vec{v}_A = \pm i I_0 \vec{v}_B, \quad \vec{v}_B = \mp i I_0 \vec{v}_A.
$$

(C9)

Thus the entries of $\vec{v}_B$ obey now the simple relation: $\sigma_{N+1-j} = \mp i \xi_j$ and a normalized eigenvector $\vec{w}$ is achieved by normalizing $\vec{v}_A$ and division by $\sqrt{2}$.

In the special case of $E = 0$, the degenerate eigenstates are still related by inversion symmetry, but the decoupling of $\vec{v}_A$ and $\vec{v}_B$ always allows to set one of them to zero whereby a relation between $\vec{v}_A$ and $\vec{v}_B$ of the same eigenvector can become invalid.

Once $\vec{v}_A$ is known, one can rewrite the solution in the basis of the fermionic operators $d_{ij}^{(t)}$. After the transformation the electron $d_j$ (hole $d_j^\dagger$) part of the quasiparticle state is $\vec{v}_A - i \vec{v}_B$ ($\vec{v}_A + i \vec{v}_B$). The different combination signals opposite behavior under inversion symmetry as captured in Fig. 3. Further, after an application of the particle-hole symmetry to the eigenstates, the character of the electron and hole parts under inversion symmetry changes into the opposite, since the exchange $E \rightarrow -E$ means $\vec{v}_B \rightarrow -\vec{v}_B$ while keeping the same $\vec{v}_A$.

2. Degenerate energy levels

The important starting point for the case of degeneracies is Fig. 2 where we see that for specific values of $t$, $\Delta$ and $\mu$ a crossing in the spectrum occurs, which naturally depends also on $N$. We consider here the case of $E \neq 0$, $t^2 \neq \Delta^2$ ($ab \neq 0$) and $t \Delta \neq 0$, because all those cases are already known. Further, we consider $t$, $\Delta$ as fixed while $\mu$ can be varied to achieve a degeneracy.

Let us begin by inspecting the degree of the degeneracy, and assume initially that we have $D \geq 2$ degenerate eigenvectors $\vec{w}^{(d)} = (\vec{v}^{(d)}, \vec{u}^{(d)})^T$ with $d = 1, \ldots , D$ and all $\vec{w}^{(d)} = (\vec{v}^{(d)}, \vec{u}^{(d)})^T$ have to obey the Eqs. (C2)-(C7). We continue with almost the same notation as above, where we change only $\xi_j$ (or $\sigma_j$) into $\xi_j^{(d)}$ ($\sigma_j^{(d)}$) for clarity. The eigenstates are still determined by the quantization rule in Eq. (6), and in the following we will obtain the required further constraint on Eq. (6) needed for the eigenstates to be degenerate.

The case of degenerate eigenvectors has to be treated carefully, since their superposition can break the connection between $\vec{v}^{(d)}$ and $\vec{u}^{(d)}$ via inversion symmetry. Nonetheless, once the value of the energy is known all information of $\vec{w}^{(d)}$ is still contained in $\vec{v}^{(d)}$, since $\vec{v}^{(d)}$ follows from $h^\dagger \vec{v}^{(d)} = E \vec{u}^{(d)}$. Furthermore, for given values of $t$, $\Delta$ and $\mu$, the functions $X_i(j)$ in Eq. (C7) differ only for states with different energy, therefore the $\vec{v}^{(d)}$ are defined only by distinct initial values $\xi_{-2}^{(d)}, \ldots , \xi_1^{(d)}$. Thus one can build and exploit special superpositions of those eigenstates yielding

$$
\begin{align*}
\xi_1^{(1)} &= 1, \quad \xi_{-2}^{(1)} = 0, \quad (C11) \\
\xi_2^{(2)} &= 0, \quad \xi_{-2}^{(2)} = 1. \quad (C12)
\end{align*}
$$

The boundary condition in Eq. (C6) demands $\xi_0^{(d)} = 0$, $\xi_{-2}^{(d)} = b \xi_2^{(d)}/a$ and thus fixes $\vec{w}^{(d)}$. Note that the Eqs. (C11), (C12) imply $D = 2$, i.e. only twofold degeneracies are allowed, since beyond $\xi_1$ and $\xi_{-2}$ there are no further degrees of freedom to exploit. As we see next, Eq. (C5) which formerly coupled $\xi_1^{(d)}$ and $\xi_{-2}^{(d)}$ becomes indeed invalid for the new superpositions. Returning to
the boundary condition in Eq. (C6), we get further constraints, namely

\begin{align}
X_{-2}(N+1) &= 0, \quad (C13) \\
\kappa_1 X_{-2}(N+2) - a X_{-2}(N) &= 0, \quad (C14) \\
\kappa_2 X_{-1}(N+1) + b X_{-1}(N+2) &= 0, \quad (C15) \\
b [a X_1(N+2) + b X_1(N+2)] - a [a X_1(N) + b X_{-1}(N)] &= 0, \quad (C16)
\end{align}

implying a division of zero by zero in Eq. (C8). Further, the Eqs. (C13) - (C16) show that the boundary condition splits into two parts for \( N + 1 \) and for \( N + 2 \), which is the constraint on Eq. (6) for which we have been looking.

We have not mentioned the wavenumbers \( \kappa_{1,2} \), or equivalently \( \kappa_{\Sigma,\Delta} = (\kappa_1 \pm \kappa_2)/2 \) so far. The definition of \( \kappa_{1,2} \in \mathbb{C} \) is implicit in \( S_{1,2} \) from Eq. (G20), as \( S_{1,2} = \pm 2 \cos(\kappa_{1,2}) \). Indeed, \( S_{1,2} = 2 \cos(\kappa_{1,2}) \) is the simplest form of the dispersion relation of the Kitaev chain in Eq. (2) and implies directly \( E(\kappa_{1,2}) = E(\kappa_{2,2}) \). Note that \( \kappa_{1,2} \) are not quantized so far. The four functions \( X_j \) are constructed with the help of two special functions \( F_{1,2} \), see Eqs. (G27) - (G30), which are nothing else than standing waves,

\[ F_{1,2}(j) = \frac{\sin((\kappa_{1,2} j))}{\sin(\kappa_{1,2})} \quad (C17) \]

at a site \( j \), constructed from the plane waves \( r_{+1,+2} = e^{i\kappa_{1,2}} \) as follows from Eqs. (G21), (G25), (G26).

Now, we can solve for \( \kappa_{1,2} \). We get first from Eq. (C13) two constraints: \( S_1 - S_2 \neq 0 \), i.e. \( \kappa_1 \neq \pm \kappa_2 \), and \( F_1(N+1) = F_2(N+1) \). Second, these two restrictions used on Eq. (C15) together with exploiting the properties of \( F_{1,2} \) (for example Eq. (G31)), give us a familiar expression, namely

\[ a X_{-2}(N+2) - b X_{-2}(N) = 0, \quad (C18) \]

which is almost Eq. (C14). Thus, \( X_{-2}(N+2) = X_{-2}(N) = 0 \) holds, or equivalently \( F_1(N+2) = F_2(N+2) \) and \( F_1(N) = F_2(N) \). This imposes a further constraint on \( \kappa_{1,2} \) to obey \( F_{1,2}(N+1) = 0 \). Thus, in principle \( \kappa_{1,2} = n \pi/(N+1) \), \( n = 1, 2, \ldots. \), \( N \).

The combinations of different values of \( \kappa_{1,2} \) yield both the positions of strict and of avoided crossings in the \((\mu, E)\) plane. The values of \( \mu \) follow from Eq. (1) after converting the values of \( \kappa_{1,2} \) into \( \kappa_{\Sigma,\Delta} \). The energy \( E \), in turn, can be obtained from the dispersion relation, either Eq. (2) or Eq. (7). Whether these \((\mu, E)\) pairs define strict or avoided crossings is determined by the general quantization rule in Eq. (6), considering the following facts. (i) With \( \kappa_{1,2} = n_{1,2} \pi/(N+1) \) the values for \( \kappa_{\Sigma,\Delta} \) are either both half-integer or both integer multiples of \( \pi/(N+1) \). (ii) The entire derivation for \( \kappa_{1,2} \) is invariant under the exchange \( \kappa_1 \leftrightarrow \kappa_2 \) and \( \kappa_1 \rightarrow -\kappa_1 \), hence, without loss of generality we can demand \( \kappa_1 > \kappa_2 \). (iii) By virtue of Eq. (5) \( \kappa_1 + \kappa_2 \neq \pi \), except for \( N \) odd and \( \mu = 0 \). In the end, we find that only \( \kappa_{\Sigma,\Delta} \) which are integer multiples of \( \pi/(N+1) \) satisfy the quantization rule (6) for arbitrary value of \( \Delta \). Thus the selection rule for strict crossings can be expressed in terms of \( \kappa_{\Sigma,\Delta} \), demanding that \( \kappa_{\Sigma,\Delta} > \kappa_{\Delta} \), and resulting in the requirement of \( \kappa_{\Sigma,\Delta} \) being integer multiples of \( \pi/(N+1) \) as stated in Eqs. (6). The half-integer multiples satisfy Eq. (6) only if \( \Delta = 0 \), hence in a superconducting chain they always define avoided crossings.

**Appendix D: Derivation of the current formula**

The electronic current (for fixed spin) in the lead is,

\[ I_L(t) = -e \langle \dot{N}_L \rangle, \quad (D1) \]

where \( e \) is the elementary charge and \( N_L = \sum_k c^\dagger_k c_k \).

The specific choice of the tunneling Hamiltonian \( H_T \) in (11) leads to the explicit expression

\[ I_L(t) = -\frac{ie}{\hbar} \sum_k \left( t_L \langle d^\dagger_k(t) c_k(t) \rangle - t^*_L \langle c^\dagger_k(t) d_k(t) \rangle \right), \quad (D2) \]

where the superconductivity is contained inside the time evolution of the creation and annihilation operators. Further, we shall use a 2×2 matrix notation for the fermionic Green’s functions (GF) whose entries are defined via \( D_j := (d_j, d_j^\dagger) \) as

\[ (G_{ij}^s(t,t'))_{nm} := -\frac{i}{\hbar} \langle (D_i(t))^n (D_j(t'))^m \rangle, \quad (D3) \]

\[ (G_{ij}^t(t,t'))_{nm} := \frac{i}{\hbar} \langle (D_j(t'))^n (D_i(t))^m \rangle, \quad (D4) \]

\[ (G_{ij}^s(t,t'))_{nm} := -\frac{i}{\hbar} \theta(t-t') \{ (D_i(t))^n, (D_j(t'))^m \}, \quad (D5) \]

\[ (G_{ij}^t(t,t'))_{nm} := \frac{i}{\hbar} \theta(t-t') \{ (D_j(t'))^n, (D_i(t))^m \}, \quad (D6) \]

where \( \{\cdot, \cdot\} \) denotes the anticommutator and \( n, m = 1, 2 \). All kinds of Green’s functions, such as \( G_{\kappa,\alpha}^s(t,t'), G_{\kappa,\alpha}^t(t,t') \) for \( s = r, a, \alpha > \), are defined analogously with \( C_{\kappa,\alpha} := (c_{\kappa,\alpha}, c_{\kappa,\alpha}^\dagger)^T \) instead of \( D_j \). Please keep in mind that the NEGF formalism uses a large variety of inter-related Green’s functions.

In the following we will denote all 2×2 matrices with a bold font, to keep them distinct from the \( 2N \times 2N \) matrices used everywhere else.

A convenient expression for the current in terms of those 2×2 matrices is

\[ I_L(t) = -e \sum_k \text{Re} \left\{ \text{Tr} \left[ \begin{pmatrix} t_L & 0 \\ 0 & t^*_L \end{pmatrix} G_{kL1}^\leq(t,t) \right] \right\}, \quad (D7) \]
Starting from the equation of motion for the relevant Green’s functions, and using standard relations between them together with the Langreth rules, we find the steady state current

$$\mathcal{I}_L = -e \int_R \frac{d\omega}{2\pi} \text{Tr} \left\{ \tau_z \left[ \Sigma^R_L(\omega) G_{11}^< \right. \right. \right.$$

$$+ \left. \left. \Sigma^<_L(\omega) G_{11}^a(\omega) \right] \right\}, \quad (D8)$$

with

$$\Sigma^R_\alpha(\omega) = \lim_{\eta \to 0} \sum_k |t_\alpha(k)|^2 \left[ \frac{1}{\hbar \omega - \epsilon_{ka} + i\eta} \right], \quad \alpha = \{ R, L \}, \quad (D9)$$

$$\Sigma^<_\alpha(\omega) = 2\pi i \sum_k |t_\alpha(k)|^2 \left[ \frac{\delta(h\omega - \epsilon_{ka})}{\delta(h\omega + \epsilon_{ka})} \right] \times$$

$$\left[ f(h\omega - eV_\alpha) \quad 0 \right] \times \left[ f(h\omega + eV_\alpha) \quad 0 \right]. \quad (D10)$$

The lesser Green’s function matrices $G_{11}^<\alpha$ involve only the first site of the Kitaev chain and carry information about the coupling of this site with both the rest of the chain and the leads. To obtain them it is convenient to work in the site-ordered particle-hole basis (cf. Eq. [B3]), where the $2 \times 2$ matrices introduced above become the building blocks of $\tilde{G}^s$ ($s = <, r, a, >$),

$$\tilde{G}^s = \begin{bmatrix} G_{11}^s & \ldots & G_{1N}^s \\ \vdots & \ddots & \vdots \\ G_{N1}^s & \ldots & G_{NN}^s \end{bmatrix}, \quad (D11)$$

We find that $\tilde{G}^r$ obeys

$$\left( \hbar \omega + i\eta \right) 1_{2N} - \tilde{H} - \tilde{\Sigma}^L - \tilde{\Sigma}^R \tilde{G}^r = 1_{2N}, \quad (D12)$$

with the self-energy matrices $\tilde{\Sigma}^L, R$ ($s = <, r, a, >$) given by

$$\tilde{\Sigma}^L_\alpha = \begin{bmatrix} \Sigma^L_\alpha & 0 & \ldots & 0 \\ 0 & 0 & \ldots & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & \Sigma^L_\alpha \end{bmatrix}_{2N \times 2N}, \quad (D13)$$

$$\tilde{\Sigma}^R_\alpha = \begin{bmatrix} 0 & 0 & \ldots & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & \Sigma^R_\alpha \end{bmatrix}_{2N \times 2N}, \quad (D14)$$

where $0$ is the $2 \times 2$ matrix filled with zeros. The Hamiltonian $\tilde{H}$ reads

$$\tilde{H} = \begin{bmatrix} -\mu \tau_z & \alpha & \alpha^\dagger \\ \alpha^\dagger & -\mu \tau_z & \alpha \\ \ldots & \ldots & \ldots \end{bmatrix}_{2N \times 2N}, \quad (D15)$$

where we kept the Pauli matrix $\tau_z$ in regular font, and the matrix $\alpha$

$$\alpha = \begin{bmatrix} -t & -\Delta \\ \Delta & t \end{bmatrix} \quad (D16)$$

accounts for nearest neighbor terms. Further, $\tilde{G}^<\alpha$ obeys

$$\tilde{G}^< = \tilde{G}^r \left[ \Sigma^L + \Sigma^R \right] \tilde{G}^s, \quad (D17)$$

with $\tilde{G}^s = \left( \tilde{G}^r \right)^\dagger$ so that all ingredients of Eq. [D8] are in principle known. The trace, and the sparsity of the self-energies $\Sigma^L, R$ allow us to express the current

$$\mathcal{I}_L = -e \int_R \frac{d\omega}{2\pi} \text{Tr} \left\{ \tau_z \left[ \Sigma^R_L(\omega) \tilde{G}^<(\omega) \right. \right.$$

$$+ \left. \Sigma^<_L(\omega) \tilde{G}^s(\omega) \right] \right\}, \quad (D18)$$

in terms of the $2N \times 2N$ matrices only. We define $\tilde{\Gamma}_\alpha := -2 \text{Im}(\Sigma^\alpha) = i(\Sigma^\alpha - \Sigma^\alpha \dagger)$ and with

$$\tilde{F}_\alpha = 1_N \otimes \left[ f(h\omega - eV_\alpha) \quad 0 \right] \left[ f(h\omega + eV_\alpha) \quad 0 \right], \quad (D19)$$

it follows that $\tilde{\Sigma}^<_\alpha = \tilde{\Gamma}_\alpha \tilde{F}_\alpha$. Since the current is a real quantity, i.e. $2\mathcal{I}_L = \mathcal{I}_L + \mathcal{I}_L^\dagger$, we find the appealing form

$$\mathcal{I}_L = \frac{ie}{2} \int_R \frac{d\omega}{2\pi} \text{Tr} \left\{ (1_N \otimes \tau_z) \tilde{\Gamma}_L \left[ \tilde{G}^< + \tilde{F}_L \left( \tilde{G}^r - \tilde{G}^a \right) \right] \right\}, \quad (D20)$$

Expressing all quantities in the default basis [B1] yields directly Eq. [13]. The corresponding expressions of the self-energies and Green’s functions are explicitly given in appendix [E].

Finding the analytical form of the conductance demands first a simplification towards Eq. [16], which mostly consists of taking the trace and using the sparsity of the self-energies. This procedure is performed at best by using Eq. [D8] and a basis transformation [B4] at the end. We find from Eq. [D17] that

$$G_{11}^< = G_{11}^r \Sigma^L_1 G_{11}^a + G_{1N}^r \Sigma^R_1 G_{N1}^a \quad (D21)$$

and Eq. [D12] yields first $\tilde{G}^r - \tilde{G}^a = -i \tilde{G}^r (\tilde{\Gamma}_L + \tilde{\Gamma}_R) \tilde{G}^a$ and thus

$$G_{11}^r - G_{11}^a = -i \left[ G_{11}^r \Gamma_L G_{11}^a + G_{1N}^r \Gamma_R G_{N1}^a \right]. \quad (D22)$$

With $2\mathcal{I}_L = \mathcal{I}_L + \mathcal{I}_L^\dagger$ it follows from Eq. [D8] that

$$\mathcal{I}_L = \frac{ie}{2} \int_R \frac{d\omega}{2\pi} \text{Tr} \left\{ \tau_z \left[ \Gamma_L G_{11}^r \Sigma^< \Gamma_L G_{11}^a \\ + \Gamma_L G_{1N}^r \Sigma^< \Gamma_R G_{N1}^a \\ - \Sigma^L \right. \left. G_{11}^r \Gamma_L G_{11}^a \\ + \Gamma_L G_{1N}^r \Sigma^< \Gamma_R G_{N1}^a \\ - \Sigma^L \right. \left. G_{1N}^r \Gamma_R G_{N1}^a \right\}, \quad (D23)$$
where the $2 \times 2$ broadening matrices read

$$\Gamma_\alpha = \begin{bmatrix} \Gamma_\alpha & 0 \\ 0 & \Gamma_\alpha^+ \end{bmatrix}$$  \hspace{1cm} (D24)

with the abbreviations $\Gamma_{\alpha}^\pm = 2\pi \sum_k |t_\alpha(k)|^2 \delta (\hbar \omega \pm \epsilon_\alpha)$. In order to shorten the expression of the trace, we define

$$f_{\alpha}^\pm := f(\hbar \omega \pm eV_\alpha)$$  \hspace{1cm} (D25)

and after a bit of algebra one finds

\[
\begin{align*}
\text{i} \, \text{Tr} \left\{ \tau_z \left[ \Gamma_L G_{11}^\ast \Sigma_L^\ast G_{11}^0 - \Sigma_L G_{11} \Gamma_L G_{11}^0 \right] \right\} &= \Gamma_{L,1}^\ast \Gamma_{R,1}^\ast \left[ |\tilde{G}_{12}^\ast(r,\omega)|^2 + |\tilde{G}_{21}^\ast(r,\omega)|^2 \right] \left[ f_{L}^\mp - f_{R}^\pm \right], \\
i \, \text{Tr} \left\{ \tau_z \left[ \Gamma_L G_{11}^\ast \Sigma_R^\ast G_{11}^0 - \Sigma_R G_{11} \Gamma_R G_{11}^0 \right] \right\} &= \Gamma_{L,1}^\ast \Gamma_{R,1}^\ast \left[ |\tilde{G}_{22}^\ast(r,\omega)|^2 \left[ f_{L}^\mp - f_{R}^\pm \right] \right. \\
&+ \Gamma_{L,1}^\ast \Gamma_{R,1}^\ast \left[ f_{L}^\pm - f_{R}^\mp \right] \\
&+ \Gamma_{L,1}^\ast \Gamma_{R,1}^\ast \left[ |\tilde{G}_{22}^\ast(r,\omega)|^2 \left[ f_{L}^\pm - f_{R}^\mp \right] \right] \\
&+ \Gamma_{L,1}^\ast \Gamma_{R,1}^\ast \left[ f_{L}^\pm - f_{R}^\mp \right].
\end{align*}
\]  \hspace{1cm} (D26)

In contrast to Eq. (16), where only electronic contributions are used, in Eqs. (D26), (D27) we have six terms for both electronic and hole degrees of freedom, and a factor of $1/2$ in front of Eq. (D23) to avoid overcounting. The following steps will further reduce the number of terms.

Throughout our approach, we considered $t$ and $\Delta$ as real quantities. Hence, $H$ is a symmetric matrix. Since $\Sigma_\alpha$ are symmetric too, we have that $G_{i,j}^\tau = G_{j,i}^\tau$. This yields in Eq. (D26) a factor of 2.

Further, the particle-hole symmetry gives

$$\left( \mathbf{1}_N \otimes \sigma_x \right) \left[ \tilde{G}^\tau(-\omega) \right]^* \left( \mathbf{1}_N \otimes \sigma_x \right) = - \tilde{G}^\tau(\omega),$$  \hspace{1cm} (D28)

where "*" denotes the complex conjugation. The use of Eq. (D28) on $\tilde{G}^\tau(\omega)$ and observing its particular action on the entries of the $2 \times 2$ block $G_{11}^\tau$ yields

$$\tilde{G}_{22}^\tau(\omega) = - \left[ \tilde{G}_{11}^\tau(-\omega) \right]^*, \hspace{1cm} (D29)$$

$$\tilde{G}_{12}^\tau(\omega) = - \left[ \tilde{G}_{22}^\tau(-\omega) \right]^*. \hspace{1cm} (D30)$$

Since $\Gamma_{\alpha}^\pm(\omega) = \Gamma_{\alpha}^\tau(-\omega)$ holds, one has simply to split the integration in Eq. (D23) into two parts. After a substitution of $\omega \rightarrow -\omega$ and the use of the relations in Eqs. (D29), (D30), we find that

$$I_L = e \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left\{ \Gamma_{L}^\tau(\omega) \Gamma_{R}^\tau(\omega) |\tilde{G}_{12}^\ast(\omega)|^2 \left[ f_{L}^\mp - f_{R}^\pm \right] \\
+ \Gamma_{L}^\tau(\omega) \Gamma_{R}^\tau(\omega) |\tilde{G}_{12}^\tau(-\omega)|^2 \left[ f_{L}^\pm - f_{R}^\mp \right] \\
+ \Gamma_{L}^\tau(\omega) \Gamma_{R}^\tau(\omega) |\tilde{G}_{12}^\ast(\omega)|^2 \left[ f_{L}^\pm - f_{R}^\mp \right] \right\} \hspace{1cm} (D31)$$

which is only separated by one final step from Eq. (16); a basis transformation given by Eq. (B54). The necessary entries of $\tilde{G}^\tau$ transform as

$$\tilde{G}_{1,2}^\tau = G_{1,N+1}^\tau,$$

$$\tilde{G}_{2,1}^\tau = G_{1,N}^\tau,$$

$$\tilde{G}_{2,2}^\tau = G_{1,2N}^\tau,$$

and inserting this in Eq. (D31) with the substitution $E = \hbar \omega$ leads almost directly to Eq. (16), though the bias still remains to be set.

The use of the mean field technique breaks the conservation of the number of particles, if fixed values of $\Delta$ are used and thus $I_L \neq -I_R$. For correctness one has to the use self-consistently calculated profile of $\Delta$, since that replaces correctly two operators with their mean values and the number of particles is (implicitly) conserved. On the other side, one obviously prefers to avoid the self-consistency cycle. After we obtain $I_R$, we find that $I_L = -I_R$ holds for symmetrically applied bias ($\eta = 1/2$, i.e. $V_L = V/2$, $V_R = -V/2$), without demanding the self-consistently calculated $\Delta$. This trick sets the internal supercurrent to zero and allows the use of fixed values of $\Delta$. As a second effect the crossed Andreev term $G_{1,2N}^\tau$ does not contribute to the current, since the difference of the Fermi functions $f_{L}^\pm - f_{R}^\mp$ is always zero for $\eta = 1/2$.

**Appendix E: Matrix expressions in the (standard) Bogoliubov de Gennes basis**

The use of the default basis $\tilde{\Psi} = (d_1, \ldots, d_N, d_1^\dagger, \ldots, d_N^\dagger)^T$ gives an intuitive understanding of the current formula, since the entries of the Hamiltonian, the self-energies and the Green’s functions are ordered first in the particle/hole subspace and second in the real space position. For example, $G_{1,N}^\tau$ describes the transport of an electron from site $j = 1$ to site $j = N$, where it leaves the Kitaev chain as an electron to the right lead. We present here the matrices used in Eq. (13). The BdG Hamiltonian $\mathcal{H}$ reads

$$\mathcal{H} = \left[ \begin{array}{cc} C & S \\ S^\dagger & -C \end{array} \right]_{2N \times 2N},$$  \hspace{1cm} (E1)
with $\hat{H}_{SC} = \frac{1}{2} \hat{\Psi}^\dagger \hat{H} \hat{\Psi}$, $\hat{H}_{SC}$ being given by Eq. [1]. The matrices $C$ and $S$ are

$$C = \begin{bmatrix}
-\mu & -t & & \\
-t & -\mu & -t & \\
& & \ddots & \ddots \\
& & & -t & -\mu & -t \\
& & & & t & -\mu & -t \\
\end{bmatrix}_{N \times N}, \quad (E2)$$

$$S = \begin{bmatrix}
0 & \Delta & & & & \\
-\Delta & 0 & \Delta & & & \\
& & \ddots & \ddots & \ddots & \\
& & & -\Delta & 0 & \Delta \\
& & & & -\Delta & 0 \\
\end{bmatrix}_{N \times N}, \quad (E3)$$

Due to the choice of the tunneling Hamiltonian $H_L$ in Eq. [11], the self-energies $\Sigma^L$ and $\Sigma^R$ are sparse matrices $(i, j = 1, \ldots, 2N)$

$$(\Sigma^L)_{i,j} = \delta_{i\ell} \delta_{j\ell} \Omega^{L-} - \delta_{N+1,i} \delta_{N+1,j} \Omega^{L+}, \quad (E4)$$

$$(\Sigma^R)_{i,j} = \delta_{i\ell} \delta_{N,j} \Omega^{R-} - \delta_{i,2N+1,j} \delta_{N+1} \Omega^{R+}, \quad (E5)$$

acting only on the first and last site. We used here the abbreviations

$$\Omega_{\alpha \pm} = \lim_{\eta \to 0} \sum_k \frac{|t_{\alpha}(k)|^2}{E + i\eta \pm \epsilon_{\alpha}}, \quad \alpha = L, R, \quad (E6)$$

where the index $-$ (+) accounts for particles (holes). In general the finite lifetime introduced by the self energies is given by the imaginary part $\text{Im}(\Omega_{\alpha \pm}) = -\pi \sum_k |t_{\alpha}(k)|^2 \delta(E \pm \epsilon_{\alpha})$. In the special case of the wide band limit the functions $\Omega_{\alpha \pm}$ don't depend on $E$ and become $\Omega_{\alpha \pm} = -i \gamma_{\alpha}$ from the main text.

Returning to the general case, the matrices $\Gamma_{\alpha}$ follow from

$$\Gamma_{\alpha}(E) = -2 \text{Im}(\Sigma^\alpha), \quad \alpha = L, R.$$

The retarded Green’s function $G^r$ is given by

$$G^r = [E\mathbb{1}_{2N} - \hat{H}_{SC} - \Sigma^L - \Sigma^R]^{-1},$$

and the advanced Green’s function obeys $G^a(E) = [G^r(E)]^\dagger$. The Fermi Dirac distribution $f(E)$ is contained in the matrix $F_\alpha$ such that

$$F_\alpha = \begin{bmatrix}
\mathbb{1}_N f(E - eV_\alpha) & \mathbb{1}_N f(E + eV_\alpha)
\end{bmatrix},$$

where $V_\alpha$ denotes the shift of the chemical potential at contact $\alpha = L, R$. Finally, the lesser Green’s function $G^<(E)$ reads

$$G^<(E) = iG^r \left[ \sum_{\alpha = L, R} F_\alpha \Gamma_{\alpha}(E) \right] G^a. \quad (E7)$$

**Appendix F: The exact form of the Green’s functions $G^r_{1,N+1}, G^r_{1,N}, G^r_{1,2N}$**

The entries of the retarded Greens function $G^r_{1,N}$ $G^r_{1,N+1}$ and $G^r_{1,2N}$ in the default basis can be obtained analytically. The calculations are most conveniently performed in the site-ordered Majorana basis defined in Eq. (B5), since the Kitaev Hamiltonian and the self energies are reshaped into a block tridiagonal matrix, see Eq. (F1) below. Keeping in mind that $G^a = T^\dagger G^r M T$, after a bit of algebra one finds that

$$G^r_{1,N+1} = \frac{1}{2} \left\{ (G^r_M)_{11} - (G^r_M)_{22} + i \left[ (G^r_M)_{12} + (G^r_M)_{21} \right] \right\},$$

$$G^r_{1,N} = \frac{1}{2} \left\{ (G^r_M)_{1,2N-1} + (G^r_M)_{2,2N} + i \left[ (G^r_M)_{1,2N-1} - (G^r_M)_{2,2N} \right] \right\},$$

$$G^r_{1,2N} = \frac{1}{2} \left\{ (G^r_M)_{1,2N} - (G^r_M)_{2,2N} + i \left[ (G^r_M)_{1,2N} + (G^r_M)_{2,2N} \right] \right\}.$$  

Although several matrix inversions are required to obtain the entries $G^r_{1,N+1}, G^r_{1,N}$ and $G^r_{1,2N}$ after the transformation, the inversion can be performed analytically. As it turns out, see Eq. (F2) below, the problem involves a non-linear combination of polynomials and the basis transformation allows the decomposition.

In the case of $N \neq 1$, the retarded Green’s function $G^r_M$ is the inverse of

$$\mathcal{M} := E \mathbb{1}_{2N} - \hat{H}_M - \Sigma^L_M - \Sigma^R_M =$$

$$= \begin{bmatrix}
A_L & B \\
C & A_2 B \\
C & A_3 B \\
& \ddots & \ddots \\
& C & A_{N-1} B \\
& C & A_R
\end{bmatrix}, \quad (F1)$$

with

$$A_j = \begin{bmatrix}
E & i\mu \\
-i\mu & E
\end{bmatrix}, \quad C^\dagger = B = \begin{bmatrix}
0 & -a \\
b & 0
\end{bmatrix},$$

$$A_\alpha = A_2 + \begin{bmatrix}
\sigma_{\alpha,p} & i\sigma_{\alpha,m} \\
-i\sigma_{\alpha,m} & \sigma_{\alpha,p}
\end{bmatrix},$$

and $j = 2, \ldots, N - 1, a = i(\Delta - t)$, $b = i(t + \Delta)$, $\sigma_{\alpha,p} = -(\alpha_{\alpha} + \alpha_{\alpha} - 2)/2, \sigma_{\alpha,m} = (\alpha_{\alpha} - \alpha_{\alpha})/2$. In the case of $N = 1$, $G^r_M$ is the inverse of

$$A_2 + \sum_{\alpha = L, R} \begin{bmatrix}
\sigma_{\alpha,p} & i\sigma_{\alpha,m} \\
-i\sigma_{\alpha,m} & \sigma_{\alpha,p}
\end{bmatrix}.$$
method explained in Ref. 62, which entails the inversion of the B-type matrices. The calculation of \( \text{det}(M) \) is straightforward, but notice that the seemingly unimportant structure of the B matrices is the key here. The matrices \( B, B^{-1} \) are off-diagonal, which avoids non-linear terms in calculating their determinants already in the beginning of the approach and is the reason to use a basis of Majorana operators. A site-ordered fermionic basis (cf. Eq. (B3)), replaces \( B \) with \( -\alpha \) from Eq. (D16) and the calculation cannot be performed easily.

Nevertheless, obtaining the entries of the adjoint matrix themselves requires even further tricks, which we cannot cover here. To give only one example: the minors of \( M \) which we have to calculate for the entries of \( G^r \) are not block tridiagonal, one column and one row is missing. One has thus to extend the matrix \( M \) to \( 2N \times 2N \) without changing the value of the determinant, while at the same time restoring the block tridiagonal shape. For the Andreev contributions one has simply to add a row and a column, which contain only zeros excepting one single "1" at position \((1,1)\) of this new matrix. Laplace’s expansion shows that the value of the determinant is unchanged, but the newly formed first upper/ lower off-diagonal block is not invertible. In order to cure this, one has to consider an entire sequence of matrices, which converge back to the former, etc. Furthermore, once this calculation is accomplished, still a different procedure has to adopted to calculate the direct and crossed Andreev terms.

We shall therefore simply give below the closed formulæ for the relevant Green’s functions, and justify their form a posteriori. For example, if one calculates first \( \text{det}(E 1_{2N} - H_M) \), which is essentially the characteristic polynomial and straightforward63 to derive with Ref. 62 one finds that

\[
\text{det}(E 1_{2N} - H_M) = (-ab)^N \left( x_N y_N - y_N \chi_N \right), \tag{F2}
\]

where the functions \( x_N, y_N, y_N, \chi_N \) are Tetranacci polynomials of order \( N \). Their name originates from their recursion formula63

\[
x_{j+2} = \frac{E^2 + a^2 + b^2 - \mu^2}{ab} x_j - x_{j-2} + i\mu \frac{b - a}{ab} \left( x_{j-1} - x_{j+1} \right), \tag{F3}
\]

which \( y_N, y_N, \chi_N \) obey too; their initial values are given in Table I. Thus, these polynomials are a generalization of Fibonacci polynomial6365. We discuss a selection of their properties in appendix C and give their closed form expression in Eq. (F23) below.

In order to generalize the result in Eq. (F2) to the case including the self-energies, one should remember that the self-energies act only on the first/last site; the interior of the matrix \( M \) in Eq. (F1) is not affected by them. Importantly, the recursion formula in Eq. (F3) is a direct consequence of this structure, which can be seen from the l.h.s. of Eq. (F2). This justifies an attempt (as it turns out, successful) to solve our problem using Tetranacci polynomials.

Following Ref. 62 one can define the polynomials \( d_j^\mu, d_j^y, d_j^= \) and \( d_j^\chi \) as a superposition of \( x_j, y_j, \chi_j \)

\[
d_j^\mu := \sigma_{R,P} x_{j-1} + i \sigma_{R,m} y_{j-1} + ay_j, \tag{F4}
\]

\[
d_j^y := \sigma_{R,P} \chi_{j-1} + i \sigma_{R,m} y_{j-1} + ay_j, \tag{F5}
\]

\[
d_j^\pi := \sigma_{R,P} y_{j-1} - i \sigma_{R,m} x_{j-1} + bx_j, \tag{F6}
\]

\[
d_j^\chi := \sigma_{R,P} \chi_{j-1} - i \sigma_{R,m} \chi_{j-1} + b\chi_j, \tag{F7}
\]

including the entries of the right self-energy as coefficients. Physical intuition leads us to believe that, similar to \( d_j^\mu, d_j^y, d_j^\pi \) also Tetranacci polynomials including only the left self-energy exist. Our use of Eqs. (F4) is only a matter of the chosen technique.

In the end, one finds

\[
\text{det}(M) (-ab)^{N-1} = d_N^\mu d_N^\pi - d_N^y d_N^\chi
\]

\[
+ \frac{\sigma_{L,m}^2 - \sigma_{L,P}^2}{ab} \left[ d_{N-1}^\mu d_{N-1}^\pi - d_{N-1}^\pi d_{N-1}^\mu \right]
\]

\[
+ \frac{\sigma_{L,P}^2}{b} \left[ d_N^\mu d_{N-1}^\mu - d_N^\pi d_{N-1}^\pi \right]
\]

\[
+ \frac{\sigma_{L,m}}{a} \left[ d_N^\mu d_{N-1}^\pi - d_N^\pi d_{N-1}^\mu \right]
\]

\[
+ \frac{i \sigma_{L,m}}{a} \left[ d_N^\pi d_{N-1}^\mu - d_N^\mu d_{N-1}^\pi \right], \tag{F8}
\]

and the entries \( G_{1,N+1}^r, G_{1,N}^r \) and \( G_{1,2N}^r \) read

\[
G_{1,N+1}^r = \frac{2\text{det}(M)}{(-ab)^N} = \frac{\mu^2}{a} \left[ d_{N-2}^\mu d_{N-1}^\pi - d_{N-1}^\pi d_{N-2}^\mu \right]
\]

\[
+ \frac{\mu^2}{b} \left[ d_{N-2}^\mu d_{N-1}^\mu - d_{N-1}^\pi d_{N-2}^\pi \right]
\]

\[
- \frac{\mu}{b} \left[ d_{N-2}^\mu d_{N-1}^\pi - d_{N-1}^\mu d_{N-2}^\pi \right]
\]

\[
- \frac{\mu}{a} \left[ d_{N-2}^\pi d_{N-1}^\mu - d_{N-1}^\mu d_{N-2}^\pi \right], \tag{F9}
\]

\[
G_{1,2N}^r = \frac{2\text{det}(M)}{(-ab)^{N-1}} = \frac{\mu^2}{a} \left[ d_{N-2}^\mu d_{N-1}^\pi - d_{N-1}^\pi d_{N-2}^\mu \right]
\]

\[
- \frac{\mu}{b} \left[ d_{N-2}^\mu d_{N-1}^\mu - d_{N-1}^\pi d_{N-2}^\pi \right]
\]

\[
+ \left( E - \Omega_{L,+} - \mu \right) \times \left[ d_{N-1}^\pi - i d_{N-1}^\mu \right]
\]

\[
- \frac{\mu}{b} \left[ d_{N-1}^\mu d_{N-2}^\mu - d_{N-2}^\pi d_{N-1}^\pi \right] \tag{F10}
\]
\[ \text{ detention } = \frac{2a}{b} \left( \frac{b}{a} \right) [d_{N-2}^x + i d_{N-2}^y] + \frac{a}{b} \left( d_{N-2}^y - i d_{N-2}^x \right) + (E - \Omega_{L,+} - \mu) \times \left[ \frac{d_{N-1}^x + i d_{N-1}^y}{b} + \frac{d_{N-1}^y - i d_{N-1}^x}{a} \right]. \]  

The results for det(\(M\)), \(G_{1,N+1}^r, G_{1,N}^r \) and \(G_{1,2N}^r \) hold for all values of \(N, t, \Delta, \mu, E\) and the wide band limit is not used yet. Notice that these functions do not diverge at \(t = \pm \Delta\), i.e. \(a = 0\) or \(b = 0\). The reason is that all denominators contain only \(a's\) and \(b's\), which are exactly canceled by the prefactors \((-ab)^{N-x}\) for \(x = 1, 2\). This statement is obvious after a look into Eq. (F1), since no entries of the matrix diverge there. Strictly speaking, one has to take the limit \(a (b) \rightarrow 0\) and not to evaluate at \(a = 0\) \((b = 0)\), but this is merely a numerical issue.

One encounters those polynomials in the calculation of the characteristic polynomial of the isolated Kitaev chain, where they obey two equivalent sets of coupled equations. The first set reads

\[ x_{j+1} = -\frac{i \mu}{b} x_j + \frac{a}{b} x_{j-1} + \frac{E}{b} y_j, \quad (G2) \]
\[ \chi_{j+1} = -\frac{i \mu}{a} \chi_j + \frac{b}{a} \chi_{j-1} + \frac{E}{a} y_j, \quad (G3) \]
\[ y_{j+1} = \frac{i \mu}{a} y_j + \frac{b}{a} y_{j-1} + \frac{E}{a} x_j, \quad (G4) \]
\[ \nu_{j+1} = \frac{i \mu}{a} \nu_j + \frac{b}{a} \nu_{j-1} + \frac{E}{a} \chi_j, \quad (G5) \]

and the second reads

\[ x_{j+1} = -\frac{i \mu}{b} x_j + \frac{a}{b} x_{j-1} + \frac{E}{a} \chi_j, \quad (G6) \]
\[ \chi_{j+1} = \frac{i \mu}{a} \chi_j + \frac{b}{a} \chi_{j-1} + \frac{E}{a} x_j, \quad (G7) \]
\[ y_{j+1} = -\frac{i \mu}{b} y_j + \frac{a}{b} y_{j-1} + \frac{E}{b} y_j, \quad (G8) \]
\[ \nu_{j+1} = \frac{i \mu}{a} \nu_j + \frac{b}{a} \nu_{j-1} + \frac{E}{b} \nu_j, \quad (G9) \]

while decoupling leads to Eq. (G1). Although the Eqs. (G2) - (G9) are equivalent to Eq. (G1), each description has its own advantages, often unseen in the other. For example, the comparison of Eq. (G2) with Eq. (G6) yields,

\[ \left( \frac{b}{a} \right) \chi_j = \left( \frac{a}{b} \right) y_j, \quad (G10) \]

and more such relationships can be found.

However, the most important reason to present Eqs. (G2) - (G9) is the limiting case of \(E = 0\), which we need to obtain the conductance formula at zero bias and temperature later. While in Eq. (G1) seemingly not much happens at \(E = 0\), in (G2) - (G9) we find that

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**Appendix G: Tetranacci polynomials and their closed formula**

1. **Definition and basic properties**

The Tetranacci polynomials \(x_j, y_j, \chi_j, \nu_j\), which we already introduced in appendix F, obey all

\[ x_{j+2} = \frac{E^2 + a^2 + b^2 - \mu^2}{ab} x_j - x_{j-2} + \frac{b - a}{ab} (x_{j-1} + x_{j+1}), \quad (G1) \]

with their initial values given in Table I. They appear at first as separated objects, but they are in fact connected by a symmetry relation. By exchanging all \(a\) terms by \(b\) terms and vice versa and turning the sign of \(\mu\) into \(-\mu\), \(x_j (\chi_j)\) transforms into \(y_j (\nu_j)\). This relationship follows from Eq. (G1) and Table I. Note also that Eq. (G1) is invariant under the inversion symmetry and exchange of \(\Delta \rightarrow -\Delta\). Further, all four polynomials carry no physical unit and \(x_j, y_j, \chi_j, \nu_j\) are real (pure imaginary) objects.

---

**Table I. The first values of the Tetranacci polynomials \(x_j, y_j, \chi_j, \nu_j\).**

| \(j\) | \(x_j\) | \(y_j\) | \(\chi_j\) | \(\nu_j\) |
|------|--------|--------|--------|--------|
| -3   | \(-\mu b\) | \(-\mu a\) | \(-E\) | \(-E\) |
| -2   | \(-b\) | \(\frac{a}{b}\) | 0 | 0 |
| -1   | 0 | 1 | 0 | 0 |
| 0    | 1 | 1 | 0 | 0 |
| 1    | \(-\mu\) | \(\mu\) | \(\frac{E}{b}\) | \(\frac{E}{a}\) |
A power law ansatz for \( x_{j,0} \propto R_j \) leads first to the values of \( R_\pm(\tilde{R}_\pm) \)

\[
R_\pm = \frac{-i\mu \pm \sqrt{4ab - \mu^2}}{2b}, \quad \tilde{R}_\pm = \frac{i\mu \pm \sqrt{4ab - \mu^2}}{2a},
\]

and a superposition of \( R^i_\pm(\tilde{R}^i_\pm) \) leads to

\[
x_{j,0} = \frac{R^{j+1}_+ - R^{j+1}_-}{R_+ - R_-}, \quad \tilde{x}_{j,0} = \frac{\tilde{R}^{j+1}_+ - \tilde{R}^{j+1}_-}{\tilde{R}_+ - \tilde{R}_-}.
\]

The similarity between \( R_\pm \) and \( \tilde{R}_\pm \) allows us to determine \( y_{j,0} \) in terms of \( x_{j,0} \)

\[
y_{j,0} = \left( -\frac{b}{a} \right)^j x_{j,0},
\]

which leads to many simplifications for the conductance formula later.

Please notice that the case of \( E = 0 \) in Eq. (G1) leads always to Fibonacci polynomials even in problems distinct from the Kitaev chain, where the Eqs. (G2) - (G9) are unknown.

A second limiting case exists for \( \mu = 0 \). We see directly from Eq. (G1), but not from the Eqs. (G2) - (G9), that \( x_{j,0}, y_{j,0}, \chi_{j,0}, \gamma_{j,0} \) show again a Fibonacci character, only of a different kind compared with the \( E = 0 \) case. Define

\[
u_j := x_{2j} / v_{2j-1}
\]

and \( \nu_{j+1} \) obeys

\[
u_{j+1} = \frac{E^2 + a^2 + b^2}{ab} \nu_j - \nu_{j-1},
\]

which mimics the form of Eq. (G11) with different coefficients and a power law ansatz gives their closed form.

From the physical point of view, the two sequences of polynomials \( u_{j+1} \) and \( v_{j+1} \) construct the Green’s functions of the \( \mu = 0 \) case, in which the Kitaev chain can be considered as two decoupled SSH-like chains.

2. The closed form of Tetranacci polynomials and their Fibonacci decomposition

We turn now to the closed formula of \( x_{j,0}, y_{j,0}, \chi_{j,0}, \gamma_{j,0} \) and \( d_{j,x}^2, d_{j,y}^2, d_{j,x}^2, d_{j,y}^2 \). The second four are a linear combination of the first four, see Eq. (F4), (F7) and hence obey Eq. (G1) too. We shall therefore derive a closed form for \( \xi_j \), a general sequence of Tetranacci polynomials obeying Eq. (G1), with arbitrary initial values \( \xi_{-2}, \xi_{-1}, \xi_0 \) and \( \xi_1 \).

The expressions for \( x_{j,0}, y_{j,0}, \chi_{j,0}, \gamma_{j,0} \) can then be obtained by inserting appropriate initial values into the formula for \( \xi_j \).

The idea is to use a power law ansatz \( \xi_j \propto r^j (r \neq 0) \) as we did in the limiting cases before. We are left to find all zeros of

\[
r^4 - \zeta r^2 + 1 - \eta (r + r^3) = 0,
\]

where we used a shorthand notation for the coefficients in Eq. (G1)

\[
\zeta := \frac{E^2 + a^2 + b^2 - \mu^2}{ab}, \quad \eta := \frac{ib - a}{ab}.
\]

One can solve for the zeros by dividing Eq. (G17) by \( r^2 \) and calling \( S = r + 1/r \) Thus, we have

\[
S^2 - 2 - \zeta - \eta S = 0,
\]

and the solutions for \( S \) read

\[
S_{1,2} = \frac{\eta \pm \sqrt{\eta^2 + 4(\zeta + 2)}}{2},
\]

Finally, we can get the zeros from \( S_{1,2} \). They read

\[
r_{\pm i} = \frac{S_i \pm \sqrt{S_i^2 - 4}}{2}, \quad i = 1, 2.
\]

The details of the connection between \( r_{\pm i} \), \( S_i \) and the dispersion relation of the isolated Kitaev chain, the wave vectors and their quantisation rule, is given in Ref. 39.

For physical intuition, the \( r_{\pm i} \) are plane waves if one uses (un)quantised wave vectors to represent them.

The ansatz for \( \xi_j \) is simply

\[
\xi_j = \sum_{i=-2}^{1} \xi_i X_i(j),
\]

where the functions \( X_i(j) \) depend only on various powers of \( r_{\pm 1}, r_{\pm 2} \), see Eq. (G27) - (G30) below, but not on the values of \( \xi_{-2} , \ldots, \xi_1 \). Hence, changing the values of \( \xi_{-2} , \ldots, \xi_1 \) does not change the functions \( X_i(j) \). As one sees directly from Eq. (G28) there are constraints on \( X_i(j) \), namely

\[
X_i(j) = \delta_{i,j}, \quad \text{for } i,j = -2, \ldots, 1.
\]
to ensure that the initial values are assumed by \( \xi_j \). One can understand Eq. (G23) as the counterpart to the Binet form, which is used to determine the closed form expression of Fibonacci polynomials (see e.g. Eq (G1)).

Despite the short form of \( \xi_j \) in Eq. (G23), the formulas of \( X_i(j) \) tend to be lengthy, such that we first introduce a short hand notation for their main pieces. We define the functions \( F_{1,2}(j) \) as

\[
F_1(j) := \frac{r_{j+1} - r_{j-1}}{r_{j+1} - r_{j-1}} = \frac{r_{j+1} - r_{j+1}^{-T}}{r_{j+1} - r_{j+1}^{-T}}, \quad (G25)
\]

\[
F_2(j) := \frac{r_{j+2} - r_{j-2}}{r_{j+2} - r_{j-2}} = \frac{r_{j+2} - r_{j+2}^{-T}}{r_{j+2} - r_{j+2}^{-T}}, \quad (G26)
\]

where the r.h.s of both equalities arise due to \( r_i r_{-i} = 1 \) for \( i = 1, 2 \). Please notice, that already \( F_{1,2}(j) \) are special solutions of Eq. (G1), since they are constructed in terms of the solutions \( r_{\pm i} \).

The polynomials \( X_i(j) \) read

\[
X_{-2}(j) = \frac{F_2(j) - F_1(j)}{S_1 - S_2}, \quad (G27)
\]

\[
X_{-1}(j) = \sum_{\sigma=1}^{2} \frac{F_\sigma(j + 2) + F_\sigma(j - 1) F_\sigma(2) - F_\sigma(3) F_\sigma(j)}{(S_1 - S_2)^2} \quad (G28)
\]

\[
X_0(j) = \sum_{\sigma=1}^{2} \frac{F_\sigma(j + 1) F_\sigma(3) - F_\sigma(j + 2) F_\sigma(2)}{(S_1 - S_2)^2} - \sum_{\sigma=1}^{2} \frac{F_\sigma(j - 1)}{(S_1 - S_2)^2}, \quad (G29)
\]

\[
X_1(j) = \sum_{\sigma=1}^{2} \frac{F_\sigma(j + 2) + F_\sigma(j) - F_\sigma(j + 1) F_\sigma(2)}{(S_1 - S_2)^2}, \quad (G30)
\]

where \( \sigma \) is meant as "not \( \sigma \)", e.g. if \( \sigma = 1 \) then we have \( \sigma = 2 \) and vice versa. As one sees, the functions \( X_i(j) \) are a superposition of the solutions \( F_{1,2}(j - x) \) (\( x = -2, -1, 0, 1 \)), such that the coefficients are sometimes \( F_{1,2}(2) \) or \( F_{1,2}(3) \). Thus, the \( X_i(j) \) are Tetranacci polynomials as well. As we saw in Eq. (G22), four initial values are required to fix a solution of Eq. (G1) and these are given with the selective property in Eq. (G24) for the \( X_i(j) \)'s. We call the \( X_i(j) \) basic or primitive Tetranacci polynomials.

A second argument that the \( X_i(j) \) obey the recursion formula in (G1), follows directly from Eq. (G23). Choosing only one initial value different from zero, e.g. \( \xi_j = \delta_{j1} \) for \( j = -2, \ldots, 1 \), results in

\[ \xi_j = X_1(j). \]

Similar choices reveal that \( \xi_j \) can be equal to only one of the \( X_i(j) \). Thus, the \( X_i(j) \) must be Tetranacci polynomials.

The easier form of \( x_{j,0} \) in Eq. (G14) cannot be seen from here, since the \( r_{\pm i} \) does not reduce to the \( R_\pm \) at \( E = 0 \). The reason is, that the recursion formulas for \( E = 0 \) and \( E \neq 0 \) do not transform directly into each other. In the limiting case of \( \mu = 0 \), we find from Eq. (G20) that

\[
S_{1|\mu=0} = -S_{2|\mu=0},
\]

yielding

\[
r_{+1|\mu=0} = -r_{-2|\mu=0}.
\]

The effect on \( F_{1,2} \) in Eqs. (G25), (G26) is

\[
F_1(j)|_{\mu=0} = (-1)^j - 1 F_2(j)|_{\mu=0},
\]

and we find further that

\[
X_{-2}(2l + 1)|_{\mu=0} = 0, \quad X_0(2l + 1)|_{\mu=0} = 0, \quad X_{-1}(2l)|_{\mu=0} = 0, \quad X_1(2l)|_{\mu=0} = 0,
\]

for all values of \( l \). Thus, the form of the recursion formula at \( \mu = 0 \) in Eq. (G1) is respected and the Tetranacci polynomials \( \xi_j \) reduce back to Fibonacci polynomials for \( \mu = 0 \).

This behavior of \( \xi_j \) can be also understood in a different way. The definition of the Tetranacci polynomial \( F_{1,2} \) is actually a so called Binet-form, i.e. the closed form of Fibonacci polynomials (see e.g. Eq. (E2)). One can easily prove that \( F_{1,2} \) obey

\[
F_i(j + 2) = S_i F_i(j + 1) - F_i(j), \quad (G31)
\]

for all \( j \), with \( F_{1,2}(0) = 0, F_{1,2}(1) = 1 \). Thus, the closed form of \( \xi_j \) can be seen as a superposition of two distinct sequences of Fibonacci polynomials \( F_{1,2} \).

However, one has to account for all four different fundamental solutions \( r_{\pm i} (i = 1, 2) \) in the case of Tetranacci polynomials. Similar to the denominator of a Binet-form, which contains the difference of the two fundamental solutions of the corresponding Fibonacci sequence \( (r_{+i} - r_{-i}) \), we find that \( S_{1,2} \) adopt this role in the case of Tetranacci polynomials. Note that \( S_1 - S_2 = r_{+1} + r_{-2} - r_{+2} - r_{-1} \).

Appendix H: Conductance formula

The conductance follows from Eq. (16) by its derivative w.r.t. the bias in the zero bias limit. In the wide band limit at \( T = 0 \)K we find

\[
G_D = 4 e^2 \frac{\gamma L \gamma R}{h} |G_{1,1,E=0}|^2, \quad (H1)
\]

\[
G_A = 4 e^2 \frac{\gamma L}{h} |G_{1,1+N,E=0}|^2, \quad (H2)
\]
and of course $G = G_D + G_A$. The necessary Green’s functions are given by the Eqs. (F8) - (F11) and we have only to evaluate them at $E = 0$. In turn one should focus first on the Tetranacci polynomials $d_0^j, d_1^j, d_2^j, d_3^j$ from Eqs. (F4) - (F7). At $E = 0$ they reduce to

$$d_0^j|_{E=0} = \gamma_R \gamma_j, 0,$$

$$d_1^j|_{E=0} = \gamma_R \gamma_j, 1, 0,$$

$$d_2^j|_{E=0} = \gamma_j, 0,$$

$$d_3^j|_{E=0} = b x_j, 0.$$

We use Eq. (G15) to eliminate $\gamma_j, 0$ and we find in a first step after some algebra that

$$\det (\mathcal{M})|_{E=0} = b^{2-2N} = b^2 x_{N, 0}^2 - x_{N, -1, 0}^2 \left( \gamma_L^2 + \gamma_R^2 \right),$$

$$+ x_{N, 0}^2 \frac{\gamma_L^2 \gamma_R^2}{b^2},$$

$$- \gamma_L \gamma_R \left( x_{N, 0}^2 - x_{N, 0} x_{N, -2, 0} \right) \times \frac{\gamma_L \gamma_R}{-abN-1},$$

$$= 0$$

(H3)

The key to shorten the last expression and to further simplifications is the function $g_s \ (s = \pm 1)$

$$g_s := b^{N-1} \left[ \frac{2}{b} x_{N, 0} + i x_{N, -1, 0} \left( \gamma_R - s \gamma_L \right) \right],$$

$$- \frac{i}{b} x_{N, 0} \gamma_L \gamma_R,$$

(H4)

since one gets that

$$-|b|^{1-N} g_s|^2 = b^2 x_{N, 0}^2 - x_{N, -1, 0}^2 \left( \gamma_R - s \gamma_L \right)^2$$

$$+ x_{N, 0}^2 \frac{\gamma_L^2 \gamma_R^2}{b^2},$$

$$- 2s \gamma_L \gamma_R x_{N, 0} x_{N, -2, 0},$$

(H5)

which is very close to the expression of $\det (\mathcal{M})|_{E=0}$ in Eq. (H3). In order to obtain the equality in Eq. (H5) one has to use that $s^2 = 1$ and that $x_{j, 0}$ is a real valued function, see Eq. (G11) and table I. The last identity we need to simplify $\det (\mathcal{M})|_{E=0}$ reads

$$x_{j, 1-0}^2 - x_{j, 0} x_{j, -2, 0} = \left( -\frac{a}{b} \right)_{j-1},$$

(H6)

which follows directly from Eq. (G14) and the fact that $R_+ R_- = a/b$ with $R_{\pm}$ from Eq. (G13). Adding and subtracting the term $2s \gamma_L \gamma_R \left( x_{N, 0}^2 - x_{N, 0} x_{N, -2, 0} \right)$ to $\det (\mathcal{M})|_{E=0}$ and using the Eqs. (H5), (H6) yields

$$\det (\mathcal{M})|_{E=0} = (-1)^N |gs|^2 - \gamma_L \gamma_R \left[ a^{N-1} + s(-b)^{N-1} \right]^2,$$

(H7)

where a factor $(-1)^{N-1}$ occurs for taking $b^{N-1}$ out of the absolute value in Eq. (H5).

Finally, the simplifications of the entries $G_{1, N}^{1, N}$ and $G_{1, N}^{1, N}$ at $E = 0$ starting from Eqs. (F9)-(F11) read

$$G_{1, 2N}^{1, N}|_{E=0} = (-1)^N a^{N-1} - (-b)^{N-1} \frac{2 \det (\mathcal{M})|_{E=0}}{g_+},$$

(H8)

$$G_{1, N}^{1, N}|_{E=0} = (-1)^{N-1} \frac{a^{N-1} + (-b)^{N-1}}{2 \det (\mathcal{M})|_{E=0}} g_-,$$

(H9)

$$G_{1, N+1}^{1, N}|_{E=0} = -i \gamma_R \frac{a^{2N-2} - b^{2N-2}}{2 \det (\mathcal{M})|_{E=0}},$$

(H10)

where we give the result of $G_{1, 2N}^{1, N}|_{E=0}$ only for completeness. The use of the Eqs. (H8) - (H10) together with Eqs. (H1) - (H2) yields to the expressions (21) - (22), as we show now.

The function $g_s$ from Eq. (19) is constructed such that $|gs|^2 = |gs|^2$. Further we have $b = ip, a = -im$ with $p = t + \Delta$ and $m = t - \Delta$. In a first step we get for the total conductance $G = G_D + G_A$

$$\frac{2 \det (\mathcal{M})|_{E=0}}{4 \gamma_L \gamma_R} \frac{\hbar}{e^2} G = \left( p^{N-1} + m^{N-1} \right) \left| g_- \right|^2 + \gamma_L \gamma_R \left( p^{2N-2} - m^{2N-2} \right)^2$$

$$+ \left( p^{N-1} + m^{N-1} \right)^2 \left[ \left| g_+ \right|^2 + \gamma_L \gamma_R \left( m^{N-1} - p^{N-1} \right)^2 \right],$$

(H11)

after reorganizing the terms arising from Eqs. (H9) - (H10). The use of Eq. (17) yields

$$|\det (\mathcal{M})|_{E=0} = \left[ |g_s|^2 + \gamma_L \gamma_R \left( m^{N-1} + s p^{N-1} \right)^2 \right]$$

and the total conductance becomes

$$G = \frac{e^2}{\hbar} \frac{\gamma_L \gamma_R \left( p^{N-1} + m^{N-1} \right)^2}{|g_+|^2 + \gamma_L \gamma_R \left( p^{N-1} + m^{N-1} \right)^2},$$

(H12)

Since $|gs|^2 = |gs|^2$ holds we find the conductance according to Eq. (18).
In the strict approach, one has to exclude that $ab = 0$ in order to arrive at the following results. The case of $ab = 0$ follows by taking the limit of $a \to 0$ and/or $b \to 0$ at the end. The full result is smooth in $a$ and $b$ as one can proof easily. However, in Ref. [62] each inversion of $B$ is countered by a multiplication with $\det(B)$ for cancellation, but both operations enter at different levels in the procedure. Hence, $ab \neq 0$ is only a technical but not a physical restriction.

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