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Multi-particle content of Majorana zero-modes in the interacting p-wave wire.

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In the topological phase of p-wave superconductors, zero-energy Majorana quasi-particle excitations can be well defined even in the presence of local density-density interactions. In this paper we examine this phenomenon from the perspective of matrix representations of the commutator $\mathcal{H} = [H, \bullet]$ with the aim of characterising the multi-particle content of the many-body Majorana mode. To do this we show that, for quadratic fermionic systems, \mathcal{H} can always be decomposed into sub-blocks that act as multi-particle generalisations of the BdG/Majorana forms that encode single-particle excitations. In this picture, density-density like interactions will break this exact excitation-number symmetry, coupling different sub-blocks and lifting degeneracies so that the eigen-operators of the commutator \mathcal{H} take the form of individual eigenstate transitions $|n\rangle\langle m|$. However, the Majorana mode is special in that zero-mode transitions are not destroyed by local interactions. It thus becomes possible to define our many-body Majoranas as the odd-parity zero-energy solutions of \mathcal{H} that minimise their excitation number. This idea forms the basis for an algorithm which is used to characterise the multi-particle excitation content of the Majorana zero modes of the one-dimensional p-wave lattice model. We find that the multi-particle content of the Majorana zero-mode operators is significant even at modest interaction strengths. We will discuss how and why these findings differ from some previous work on the structure of the Majorana operators in the presence of interactions.

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I. INTRODUCTION

Zero-energy Majorana quasi-particles are expected to be pinned to defects and/or domain walls in topological superconductors.^{1,2} These particles are predicted to display fractionalised non-abelian statistics, which may allow for the manipulation quantum information in a robust manner using non-local braiding operations.³⁻⁵ There are now a number of potential systems in which these Majorana modes could potentially be observed,⁶⁻⁸ the most well-known being those based on proximity-coupled semiconductor nano-wires.^{9,10} In these nano-wire systems, observations of anomalous zero-bias conductances are a strong experimental indication of the Majorana modes.¹¹⁻¹³ More recently, alternative approaches using magnetic molecules, whose bound states can be resolved energetically and spatially, have also attracted interest.¹⁴

On a mean-field level, the notion of Majorana quasi-particle has proved enormously useful as both a conceptual and calculational tool. There is therefore ample reason to explore how much of this quasi-particle picture remains valid beyond the confines of mean-field superconductivity. For example, there has been considerable progress made towards developing number preserving theories of the Majorana modes,¹⁵⁻²⁰ as well as a growing body of work which examines how free-topological superconducting phases are affected by the addition of interacting electron-electron terms.²¹⁻³³ One aspect of this latter story is concerned with the stability and structure of the Majorana zero-modes themselves and how they are affected by the presence of density-density interaction terms that break the exactly solvable nature of the underlying model. This story of stable zero-modes has also been addressed in the related context of 1-d parafermionic chains.³⁴⁻³⁶

To make the following discussion precise, note that in the topological phase of the 1-dimensional p-wave superconducting wires the Majorana modes/operators are exponentially lo-

calised at each end of the wire.² In the limit $N_x \rightarrow \infty$ the (L)eft and (R)ight Majorana modes have precisely the energy $E = 0$ and the corresponding operators can have the form

$$\begin{aligned}\gamma_L &= \sum_i^{N_x} i(c_i^\dagger - c_i)u_L(i) \\ \gamma_R &= \sum_i^{N_x} (c_i^\dagger - c_i)u_R(i)\end{aligned}\quad (1)$$

where $u_L(i)$ and $u_R(i)$ are the single particle wave-functions localised to the left and right of the wire, and the c^\dagger 's and c 's are the Dirac fermion creation and annihilation operators respectively. For free-fermionic systems the existence of these zero-energy solutions can be easily established throughout the topological region.² It is important to note that the mode stability has nothing to do with any rigidity in the form of the functions u_L and u_R . Indeed, the functions themselves are actually very susceptible to variations in the underlying system and it is this fluidity that allows the zero-energy Majorana modes to exist even in highly disordered regions of the topological phase, see for example Ref. 37.

The zero-mode operators γ_L and γ_R commute with the Hamiltonian $[H, \gamma_{L/R}] = 0$, anti-commute with both parity P and each other ($\{P, \gamma\} = 0$, $\{\gamma_L, \gamma_R\} = 0$), and are self adjoint $\gamma_{L/R}^2 = I$. When interactions are included, and if they exist, the zero-energy Majorana modes should obey the same criteria but should now appear in the form of multi-nomial sums:²⁵

$$\begin{aligned}\gamma_L &= \sum_i^{2N_x} u_L^{(1)}(i)\gamma_i + \sum_{ijk}^{2N_x} u_L^{(3)}(i, j, k)\gamma_i\gamma_j\gamma_k + \dots \\ \gamma_R &= \sum_i^{2N_x} u_R^{(1)}(i)\gamma_i + \sum_{ijk}^{2N_x} u_R^{(3)}(i, j, k)\gamma_i\gamma_j\gamma_k + \dots\end{aligned}\quad (2)$$

where $\gamma_{2i-1} = c_i^\dagger + c_i$ and $\gamma_{2i} = i(c_i^\dagger - c_i)$.

Establishing the existence of multi-particle modes outside of the context of mean-field superconductivity has not been straightforward. Refs. 25 and 26 addressed this issue on a general level and showed that, provided only an odd number of Majorana modes participate in the Hamiltonian, interacting zero-modes of the type above can always be well defined in the presence of local parity-preserving interacting terms. These papers suggest that the multi-particle content of these modes should be significant and demonstrate how the notion of a zero-mode can survive when the system is coupled to additional bosonic degrees of freedom. This can then be used to describe in what way the generalised parity based qubits (see e.g. Ref. 38) are susceptible to thermal noise.

The question of existence was also addressed in the specific context of one-dimensional wires. In Ref. 23 it was shown that, when the p-wave system can be bosonized, a further refermionization argument can be made that indicates the continued stability of the modes in interacting regions of the topological phase. Importantly, this argument does not require the restriction to an odd number of Majorana modes.

The re-fermionization procedure casts the many-body Majorana operator in a form that resembles a renormalised single-particle wavefunction of the form Eq. (1). Although this allows us to examine general features that the operator in a single-particle picture, it does not imply that the many-body contributions to the operator ($u^{(3)}$, $u^{(5)}$ etc.) are suppressed. This is an important point because in related work on the proximity coupled semi-conductor model,²⁴ calculations of the weights of the linear ground-state cross-correlators, obtained using DMRG/MPS techniques, do actually indicate that the many-body Majorana operators resemble renormalised non-interacting modes, even in the presence of strong interactions.

The main observation of Ref. 31 was that the long wire limit of the Kitaev chain model, when in the topological phase, all eigenstates come in degenerate pairs even in the presence of local interactions. A general definition of the many-body Majorana operators follows:

$$\begin{aligned}\gamma_R &= \sum_n |n_e\rangle\langle n_o| + |n_o\rangle\langle n_e| \\ \gamma_L &= i \sum_n |n_e\rangle\langle n_o| - |n_o\rangle\langle n_e|\end{aligned}\quad (3)$$

where the states $|n_o\rangle$ and $|n_e\rangle$ are the odd and even eigenstates of the Hamiltonian. This result established that the Majorana modes are well defined throughout the whole topological region without the a-priori restriction on the numbers of the participating Majorana modes in the defining Hamiltonian, or the requirement that the chemical potential be far from the bottom of the band.

In this current paper we set out to characterise the many-body zero modes of the generic 1-d p-wave interacting model by numerically calculating the weights

$$|N_n^\Gamma|^2 = \int |u_{L/R}^{(n)}(\vec{x})|^2 d\vec{x} \quad (4)$$

where the weights have the property that $\sum |N_n^\Gamma|^2 = 1$. In-

stead of essentially single particle structure found in Ref. 24, we find that higher N-particle terms actually grow quickly as one increases the interaction strength U . More specifically we find that

$$\begin{aligned}|N_3^\Gamma(U)| &\propto \alpha_3 U \\ |N_5^\Gamma(U)| &\propto \alpha_5 U^2 \\ |N_7^\Gamma(U)| &\propto \alpha_7 U^3 \\ &\vdots\end{aligned}\quad (5)$$

The linear dependence of $|N_3^\Gamma|$ on U results in many-particle participation rates that are quite significant even at modest interaction strengths. We will discuss this discrepancy with Ref. 24 in much more detail later but note here that it largely follows from different operational definitions of the Majorana quasi-particles in the interacting regime. While we are interested in computing the *unique* operators $\gamma_{L/R}$ which take every eigenstate to its degenerate parity-swapped counterpart, the approach of Ref. 24 uses a less restrictive notion, where one seeks to quantify how well the two degenerate ground-states may be mapped into each other using the set of single particle operators. More specifically they calculate

$$|N_1^{\text{gs}}|^2 = \int |O_x|^2 dx, \quad (6)$$

where $O(x) = {}_e\langle 0 | c_x^\dagger \pm c_x | 0 \rangle_o$. This measure tends to stay very close to unity even at extremely high interaction strengths (see Figure 4). However, aside from the non-interacting regime, this approach does not allow one to *uniquely* determine the single particle content of the Majorana mode. Indeed, as we will show, the measure O_x generically includes contributions from the higher N-particle parts of the Majorana operator, and hence it is not a reliable measure to use in this specific instance. This aspect of the story has relevance to the ongoing discussion on the relative merits of what are called weak and strong zero-modes.^{39,40} The results of this paper show that when interactions are present, it is typically impossible to infer the structure of the unique strong zero-modes from the properties of the ground-state manifold. This has direct consequences for how we should interpret experimental measurements, which typically only probe the low-energy states.

The paper is structured as follows. In section II A we show how to arrive at operator representations of the commutator $[H, \bullet]$. This discussion clarifies the relationship between commutator approach of Refs. 25 and 26 and the degeneracy methodology of Ref. 31. In II B we show that in the representation generated by the position space Majorana operators, the non-interacting model commutator $[H, \bullet]$ naturally decomposes into blocks spanned by fermionic transitions of the same number. In section II C we show how one can understand the relationship between single-particle excitations and the individual energy transitions at the commutator level. In section II D we build on this idea and show how to relate the notion of integrability in quadratic systems and hopping and pairing symmetries in a fermionic model made from two copies of the original. There are similarities between this ap-

proach and the iterative methods to find parfermionic zero-modes (see for example Ref. 34). In section IIE we give a spin-representation for the Kitaev chain commutator, in which the basis states are transparently related to the differences in fermionic occupation.

The results of section II are also used to show that many-body Majorana quasi-particles (3) are the odd parity zero-modes that minimise their total transition number. This latter idea forms the basis for an algorithm outlined in section III to calculate the many-body zero-mode solutions for larger system sizes than are possible with the exact diagonalization method of Ref. 31. In section IV we discuss the resulting numerical data, focusing in particular on the N-particle participation rates mentioned in Eq. (5). We also present additional analysis of the how the multi-particle content grow with respect to the other parameters of the model noting in particular the clear parabolic dependence of α_n around $\mu = 2t$, where we have linear dispersion. In section V we discuss why ground state correlators will necessarily underestimate the many-particle contributions to the Majorana zero-mode in the presence of interactions.

We also include a number of appendices to help make this paper more self contained. In appendix A we briefly review the p-wave Hamiltonian. In appendix B we show how to derive a spin-representation using the algebra of position space Majorana operators. This basis is naturally block diagonal for quadratic Hamiltonians. In appendix C we show how to derive a spin representation using the algebra of position space fermionic creation and annihilation operators. This basis shows us how the commutator $[H, \bullet]$ can be thought of as a doubled fermionic system and how the symmetry responsible for the aforementioned block decomposition can be understood as fermionic hoppings or pairings between each copy. In appendix D we review the full diagonalisation methodology outlined in Ref. 31 which is used to benchmark the commutator algorithm of section III. In appendix E we outline some additional numerical results and in appendix F we discuss the possibility of using sub-sets of operators to represent the mappings between ground states.

II. COMMUTATOR REPRESENTATIONS, QUADRATIC HAMILTONIANS, AND CONSERVATION OF TRANSITION NUMBER

The central aim of this section is to show how the zero-mode solutions of the Hamiltonian commutator $[H, \gamma_{L/R}] = 0$, (see for example Refs. 25 and 26), are related to the arguments that establish the Majorana mode stability by proving the universal even-odd degeneracy for all eigenstates of the model.³¹ In section IIA we show how transitions between energy eigenstates are always eigen-operators of the commutator $\mathcal{H} = [H, \bullet]$, and discuss formally how to give a matrix representation to the commutator. In section IIB we show how to derive a matrix representation for the commutator using the Majorana position space operators and in IIC demonstrate that when H is quadratic, this matrix-representation block diagonalises into sub-matrices in which the conserved

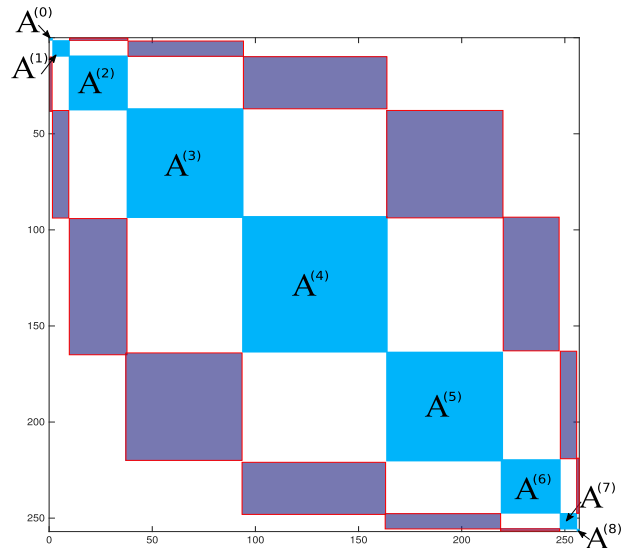


FIG. 1. The commutator \mathcal{H} for a quadratic fermion model can be decomposed into blocks $A^{(s)}$ which encode energy transitions involving the same number of fermions s . In this example we show the $2N + 1$ blocks due to an $N = 4$ fermion model. Quartic interacting terms (dark-blue/purple) connect different $A^{(s)}$ blocks, breaking the symmetry responsible for the excitation number conservation.

quantity is the number of fermions involved in a transition. In this picture, density-density like interactions will break this exact excitation-number symmetry, coupling different sub-blocks together. This results in a lifting of degeneracies so that the eigen-operators of the commutator \mathcal{H} can only take the form of individual transitions $|n\rangle\langle m|$. In section IID we discuss the symmetry operator responsible for excitation number conservation, showing that in the Majorana basis it counts fermion number and that it can also be understood as a sum of hopping or pairing terms between two related copies of the original Hamiltonian. In section IIE we outline a spin-representation for the Kitaev chain commutator that is block-diagonal.

A. Operator inner products and representations of the commutator

Suppose $|n\rangle$ is an orthonormal basis for a Hilbert space then we can decompose any operator \hat{X} as

$$\hat{X} = \sum_{nm} |n\rangle\langle n|\hat{X}|m\rangle\langle m| = \sum_{nm} \langle n|\hat{X}|m\rangle |n\rangle\langle m| \quad (7)$$

Using the Hilbert-Schmidt or operator inner-product

$$(A|_B) = \frac{\text{Tr}(A^\dagger B)}{\sqrt{\text{Tr}(A^\dagger A) \text{Tr}(B^\dagger B)}} \quad (8)$$

we have $(|n\rangle\langle m|_B) = \text{Tr}(|m\rangle\langle n|\hat{X}) = \langle n|\hat{X}|m\rangle$ and we can rewrite the operator decomposition in a generalised Dirac

vector space notation:

$$\left| \hat{X} \right\rangle = \sum_{nm} (|n\rangle\langle m| \left| \hat{X} \right\rangle |n\rangle\langle m|) \quad (9)$$

where the basis states are labeled by operators.

If we introduce a set of orthonormal vectors $(\Psi_i \left| \right.$ such that $(\Psi_i \left| \Psi_j) = \delta_{ij}$ we can, by using the cyclic properties of the trace, also provide a representation for more general operations such as commutators:

$$\begin{aligned} \mathcal{X}_{ij} &= \left(\Psi_i \left| [X, \bullet] \left| \Psi_j \right. \right) \quad (10) \\ &= \left(\Psi_i \left| [X, \Psi_j] \right. \right) = - \left([\Psi_i, X^\dagger] \left| \Psi_j \right. \right) \\ &= (\Psi_i \left| X \Psi_j) - (\Psi_i X^\dagger \left| \Psi_j) \\ &= (\Psi_i \left| X^R - X^L \left| \Psi_j) \end{aligned}$$

where, to give a matrix representation to the operator X^L we should consider its action to the left. Note that in this case the conjugate of the X appears to the right of what ever is inside $(\Psi_i \left| \right.$. We can use the above procedure to define the transition Hamiltonian matrix

$$\begin{aligned} \mathcal{H}_{ij} &= \left(\Psi_i \left| [H, \bullet] \left| \Psi_j \right. \right) \quad (11) \\ &= (\Psi_i \left| H \Psi_j) - (\Psi_i H^\dagger \left| \Psi_j) \\ &= -(\Psi_i \left| H^L - H^R \left| \Psi_j) \end{aligned}$$

In this definition the operators Ψ are labels for vectors within a enlarged Hilbert space where the matrix \mathcal{H} encodes all possible transitions between all eigenstates of the usual Hamiltonian H . To see this note that if $|n\rangle$ are the eigenstates of the Hamiltonian ($H|n\rangle = E_n|n\rangle$) then outer products $\omega_{nm} = |n\rangle\langle m|$ are orthonormal eigen-operators of the commutator with eigenvalues $E_n - E_m$. This can be easily seen from direct calculations

$$\begin{aligned} [H, \bullet] |n\rangle\langle m| &= [E_n - E_m] |n\rangle\langle m| \quad (12) \\ \text{Tr}(|l\rangle\langle k|n\rangle\langle m|) &= \delta_{nk}\delta_{ml} \end{aligned}$$

To see this using the the operator inner-product notation introduced above, note that:

$$\begin{aligned} \mathcal{H}_{nm,kl} &= -(|n\rangle\langle m| \left| H^L - H^R \left| |k\rangle\langle l| \right. \right) \quad (13) \\ &= -(|n\rangle\langle m| \left| E_m - E_k \left| |k\rangle\langle l| \right. \right) \\ &= (E_k - E_m)\delta_{nk}\delta_{ml} \end{aligned}$$

Clearly then transition outer products are eigenstates of the commutator $[H, \bullet]$ and this does not depend on the Hamiltonian being quadratic. However, for free quadratic systems there will be many eigenstates $|n\rangle\langle m|$ with the same eigenvalues $(E_n - E_m)$ and a single *quasi-particle* excitation with energy $\epsilon = E_n - E_m$ can be understood then as a particular superposition of these degenerate outer-products $|n\rangle\langle m|$. In this light we see that the Majorana quasi-particles in Eq. 3 are a specific example of this where all $E_n - E_m$ go to zero.

The central result of Ref. 31 is that this universal even-odd degeneracy remains even in the presence of interactions and therefore there is a well defined and unique definition of the Majorana zero-mode operators throughout the topological region.

B. A operator basis with Majoranas

In this section we show how by using the fermionic algebra for Majorana fermions we can construct an orthogonal basis for the commutator Hilbert space. For more details readers should consult Ref. 25. Setting

$$p_n = \gamma_{2n-1} = c_n^\dagger + c_n, \quad m_n = \gamma_{2n} = i(c_n^\dagger - c_n) \quad (14)$$

which obey the algebra $\{\gamma_i, \gamma_j\} = 2\delta_{ij}$ and thus $\gamma_i = \gamma_i^\dagger$ and $\gamma_i^2 = I$. If N is the number of unique fermion modes in our system, using these root operators we can then construct a full set of orthogonal operators:

$$\begin{aligned} \Gamma^{(0)} &: I \quad (15) \\ \Gamma^{(1)} &: \gamma_1, \gamma_2, \gamma_3, \dots, \gamma_{2N}, \\ \Gamma^{(2)} &: i\gamma_1\gamma_2, i\gamma_1\gamma_3, \dots, i\gamma_{2N}\gamma_{2N-1}, \\ \Gamma^{(3)} &: -i\gamma_1\gamma_2\gamma_3, \dots, -i\gamma_{2N-2}\gamma_{2N-1}\gamma_{2N}, \\ &\vdots \\ \Gamma^{(2N)} &: i^{(2N)N} \gamma_1\gamma_2 \dots \gamma_{2N}. \end{aligned}$$

We will denote each operator by Γ_a , for $a = 1, \dots, 2^{2N}$. For each a one then defines s to be the number of γ 's in the product Γ_a . In each of these subsets there are $\binom{2N}{s}$ elements and when we need to refer to a particular element of the subset s we will write $\Gamma_a^{(s)}$. It may occasionally be convenient to also use the notation $m_x = \Gamma_x^{(m)}$ and $p_x = \Gamma_x^{(p)}$ to refer to the specific types of $\Gamma_x^{(1)}$ terms. The phases are chosen so that $\Gamma_a^2 = I$ and since the product of two Γ_a 's gives a third (up to a phase) and $\text{Tr}(\Gamma_a^{(s)}) = 0$ for $s > 1$ then we have

$$(\Gamma_a \left| \Gamma_b) \equiv \text{Tr}(\Gamma_a^\dagger \Gamma_b) / 2^{2N} = \delta_{ab} \quad (16)$$

In Appendix C we show that one can define an orthonormal operator basis with complex fermions in a similar way to how we defined Γ_a above using the algebra of the γ terms. We will see that this constructions allows one to map our transition-Hamiltonian matrix to a normal fermionic system composed of two copies of the original Hamiltonian, allowing one to understand many properties of commutator $[H, \bullet]$, including the symmetries responsible for its block diagonal structure of non-interacting models, in terms of hoppings and pairings between these two copies. Furthermore, complex fermions representations reason are crucial to understanding how the block structure of the transition matrix \mathcal{H} when written in the Γ basis, is related to the single-particle transitions when the Hamiltonian H is quadratic. We will discuss this aspect in detail in next section II C.

C. Quadratic Hamiltonians and Block diagonal Commutators

A generic quadratic free-fermion Hamiltonian can be written as

$$H_Q = \frac{1}{2} \sum_{i,j=1}^N A_{ij}^{(1)} \gamma_i \gamma_j \quad (17)$$

where $A_{ij}^{(1)} = -A_{ji}^{(1)}$ is a pure imaginary number. For free fermionic systems it is sufficient to diagonalise the matrix $A^{(1)}$ to be able to write down expressions for all eigenstates of the Hamiltonian. This is because the eigensolutions of this block represent the single excitations of the free fermionic system:

$$H_Q = \frac{1}{2} \sum_i \epsilon_i (\lambda_i^\dagger \lambda_i - \lambda_i \lambda_i^\dagger) \quad (18)$$

with

$$\lambda_i^\dagger = \sum_{j=1}^{2N} V_{ij}^* \gamma_j, \quad \lambda_i = \sum_{j=1}^{2N} V_{ij} \gamma_j. \quad (19)$$

The ground state of the system is defined to be the state with zero occupancy of all modes and all higher energy eigenstates of can also be defined by filling some or all of these modes.

By direct computation using Eqs. (8), (11) and (17), the transition Hamiltonian matrix

$$\mathcal{H}_{ab}^\Gamma = \left(\Gamma_a \left[H_Q, \bullet \right] \Gamma_b \right) \quad (20)$$

can be easily seen to be block diagonal in each of the unique sub-blocks consisting of a 's and b 's with the same s . The simplest non-trivial example is the $s = 1$ sub-block, which is actually the $2N \times 2N$ adjacency matrix $A^{(1)}$ used to define the Hamiltonian in Eq. (17) (see Ref. 25).

It is helpful to note how \mathcal{H} looks in the complex λ -fermion basis generated from $I = \lambda_n^\dagger \lambda_n + \lambda_n \lambda_n^\dagger$, λ_n , λ_n^\dagger and $Z_n^{(\lambda)} = \lambda_n^\dagger \lambda_n - \lambda_n \lambda_n^\dagger$. We will refer to generic combinations of these λ -terms as Λ_a where we again assume a normalisation such that $(\Lambda_n | \Lambda_m) = \delta_{nm}$. In this case, the matrix is diagonal:

$$\mathcal{H}_{ab}^\Lambda = (\Lambda_a | [H_Q, \bullet] | \Lambda_b) = \delta_{ab} E_a \quad (21)$$

where E_a is a weighted sum over energies $\pm \epsilon_n$ for each unpaired λ_n^\dagger and λ_n occurring in the element Λ_a :

$$E_a = \sum_{\lambda_i^\dagger \in \Lambda_a} \epsilon_i - \sum_{\lambda_i \in \Lambda_a} \epsilon_i \quad (22)$$

The states $| \Lambda_a \rangle$ labeled with λ_n^\dagger , λ_n , I_n or Z_n can be identified with eigenstates of just one of the $A^{(s)}$ sub-blocks. However if we use the basis set λ_n^\dagger , λ_n , $\lambda_n^\dagger \lambda_n$ and $\lambda_n \lambda_n^\dagger$ this is not the case. To illustrate this we consider the example of the state $| \Lambda_a \rangle = | \lambda_1^\dagger, \lambda_2, Z_3, I_4 \rangle$ which is a transition energy

eigenstate of the $A^{(4)}$ block with an energy $\epsilon_1 - \epsilon_2$. Importantly this state can be written as a superposition of two states

$$\begin{aligned} | \Lambda_a \rangle &= | \lambda_1^\dagger, \lambda_2, Z_3, I_4 \rangle \\ &= | \lambda_1^\dagger, \lambda_2, \lambda_3^\dagger \lambda_3 - \lambda_3 \lambda_3^\dagger, I_4 \rangle \\ &= \frac{1}{\sqrt{2}} (| \lambda_1^\dagger, \lambda_2, \lambda_3^\dagger \lambda_3, I_4 \rangle - | \lambda_1^\dagger, \lambda_2, \lambda_3 \lambda_3^\dagger, I_4 \rangle) \end{aligned} \quad (23)$$

which both have support on the $A^{(2)}$ and $A^{(4)}$ sectors. When brought together with a negative sign like this, the parts of the wave-function in the $A^{(2)}$ sector cancel and we are left with only the part of the state in the $A^{(4)}$ sub-block. On the other hand suppose we bring these states together with a positive sign. In this case we have

$$\begin{aligned} | \Lambda_a \rangle &= \frac{1}{\sqrt{2}} (| \lambda_1^\dagger, \lambda_2, \lambda_3^\dagger \lambda_3, I_4 \rangle + | \lambda_1^\dagger, \lambda_2, \lambda_3 \lambda_3^\dagger, I_4 \rangle) \\ &= | \lambda_1^\dagger, \lambda_2, \lambda_3^\dagger \lambda_3 + \lambda_3 \lambda_3^\dagger, I_4 \rangle \\ &= | \lambda_1^\dagger, \lambda_2, I_3, I_4 \rangle \end{aligned} \quad (24)$$

which is entirely supported by the $A^{(2)}$ block.

In section II A we noted that the eigen-operators of \mathcal{H} are the outer-products $| n \rangle \langle m |$ and that the eigenvalues are $E_m - E_n$. However, if the fermionic system is quadratic, we can also solve in each of the $A^{(s)}$ sub-blocks separately and we know that we can interpret the solutions of the single-particle sub-block $A^{(s)}$ as operators which act across the full Hilbert space. To see how these two pictures are related we need to understand exactly what is happening in all sub-blocks.

The solutions of the $A^{(1)}$ sub-block represent all possible transitions between states which differ by the occupancy of a single λ_i or λ_i^\dagger mode. The excitation energies $\pm \epsilon_i$ therefore correspond to the energy difference $\pm (E_n - E_m)$ between any two such states. Importantly because this sub-block this spanned only by elements $| \gamma_1, I_2, I_3, \dots, I_N \rangle$, $| I_1, \gamma_2, I_3, \dots, I_N \rangle$ etc. that have only single the entries of γ combined with I 's on all other sites, we write our eigensolutions of this block as (e.g $| \lambda_1^\dagger, I_2, I_3, \dots, I_N \rangle$, $| I_1, \lambda_2, I_3, \dots, I_N \rangle$ etc. with energies $\epsilon_1, -\epsilon_2$ resp.) in a similar fashion.

In the more general cases of odd valued s , we see that the transition energies of the state $| \Lambda_a \rangle$ only depend on the number of unpaired λ_i^\dagger 's and λ_i 's and therefore states like $| \lambda_1, Z_2, I \dots I \rangle$, $| \lambda_1, I, Z_3 \dots I \rangle$, $| \lambda_1, Z_2, \dots, Z_N \rangle$, etc. all have energy $-\epsilon_1$. They are therefore degenerate with the $-\epsilon_1$ state which is contained fully within the $A^{(1)}$ sector. In each sector there are $\binom{N-1}{(s-1)/2}$ states with the same energy as the single particle transition ϵ_1 and therefore associated with a unique excitation λ_1 , we have total of

$$\sum_{s \in \text{odd}} \binom{N-1}{\frac{s-1}{2}} = 2^{N-1} \quad (25)$$

transitions.

Recall now our original eigenbasis states $|n\rangle$. In the eigenbasis provided by single particle λ_i fermion states we may associate each state n with a Fock representation such that

$$|n\rangle = |n_1, n_2, n_3, \dots, n_N\rangle \quad (26)$$

is given by the binary occupation number of the fermionic levels λ_i . Using (C1) this means for example that, we can write an individual outer-product transition

$$|10\dots 1\rangle\langle 00\dots 1| = |1\rangle\langle 0| \otimes |0\rangle\langle 0| \dots \otimes |1\rangle\langle 1|,$$

as

$$|\lambda_1^\dagger, \lambda_2 \lambda_2^\dagger, \dots, \lambda_N^\dagger \lambda_N\rangle \quad (27)$$

Again we stress that although this transition is an eigenstate with the energy ϵ_1 , it is not the same as the state $|\lambda_1^\dagger, I_2, \dots, I_N\rangle$ which represents the actual free λ_1^\dagger transition that we calculate by diagonalising the $A^{(1)}$ block which encodes the BdG/Kastelyn matrix forms.

D. Symmetries and hopping/pairing

The Hamiltonians we study in this paper all conserve fermionic parity. That is, each term appearing in the Hamiltonian, is constructed from a product of an even number of fermionic terms. This means that the transition Hamiltonian $\mathcal{H} = [H, \bullet]$ can always be decomposed into two sectors: an odd sector and an even sector. This parity conservation is due to a symmetry

$$\mathcal{P} = \prod_j p_j^L m_j^L p_j^R m_j^R = P^L P^R \quad (28)$$

where P^L is the parity operator for H^L and P^R is the parity operator for H^R .

When the system is strictly quadratic, each of these excitation-parity sectors can be further decomposed into smaller blocks which are spanned by basis states $|\Gamma^{(s)}\rangle$. This block diagonal structure exists because of a symmetry of the commutator \mathcal{H} in which the conserved quantity is the total number of particle excitations and de-excitations e.g. the eigensolutions of the $A^{(1)}$ block represent all possible single particle transitions, the solutions of the $A^{(2)}$ all double transitions etc.). The operator responsible should commute with the \mathcal{H} and, if well chosen, count the number of unique γ terms in each basis state $|\Gamma\rangle$. Working under the assumption that left and right acting operators are mutually fermionic, the symmetry operator \mathcal{N} then in this case is

$$\begin{aligned} \mathcal{N} &= \sum_{j=1}^N I + \frac{i}{2} (p_j^L p_j^R - m_j^L m_j^R) \\ &= \sum_{j=1}^N I - \frac{i}{2} (c_j^{\dagger L} c_j^{\dagger R} + c_j^L c_j^R). \end{aligned} \quad (29)$$

We can easily see that this operator does indeed count the number of excitations using the spin representation outlined in section B where we see that each term in the above summation locally looks like

$$\frac{2I \otimes I - I \otimes \sigma^z + \sigma^z \otimes I}{2} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix} \quad (30)$$

where the basis states are given by Eq. (B7).

E. A block-diagonal spin representation for the Kitaev chain commutator $[H, \bullet]$

Using the basis Γ -basis outlined in Appendix B we can write the commutator $[H, \bullet]$ for the 1-d p -wave chain (see section A) as:

$$\begin{aligned} \mathcal{H}_Q &= \frac{u_l}{2} \sum_j (\sigma_{2j-1}^x \sigma_{2j}^y - \sigma_{2j-1}^y \sigma_{2j}^x) \\ &+ \frac{t + \Delta}{2} \sum_j (\sigma_{2j}^y \sigma_{2j+1}^x - \sigma_{2j}^x \sigma_{2j+1}^y) \\ &+ \frac{t - \Delta}{2} \sum_j \sigma_{2j}^z \sigma_{2j+1}^z (\sigma_{2j-1}^x \sigma_{2j+2}^y - \sigma_{2j-1}^y \sigma_{2j+2}^x) \end{aligned} \quad (31)$$

and

$$\mathcal{H}_I = \frac{U}{8} \sum_j (\sigma_{2j-1}^x \sigma_{2j}^y \sigma_{2j+1}^x \sigma_{2j+2}^y - \sigma_{2j-1}^y \sigma_{2j}^x \sigma_{2j+1}^y \sigma_{2j+2}^x) \quad (32)$$

The matrix $\mathcal{H}_Q = [H, \bullet]$ decomposes into blocks that count the overall excitation number, see Appendix II D. Note that the spin-representation used above is by no means unique but we use this one because in this basis the symmetry \mathcal{N} is diagonal and there is a direct relationship between the binary indexing of the basis elements and the precise form of Γ_a . For example, state $|m_1\rangle$ has a binary index 100...000, $|p_1\rangle$ has a binary index 010...000, and $|Z_N\rangle$ has the index 000...0011. This makes it easy to interpret the meaning of the eigenstates of \mathcal{H} .

In section II C we discussed how the actual eigenstates of the commutator \mathcal{H}_Q , which encode all transitions in our free system, are related to solutions obtained by diagonalising each block separately. Indeed, as is well understood, for a quadratic system we only need to focus on the $A^{(1)}$ sub-block which is just a representation of the original adjacent matrix used to define the full Hamiltonian. However the actual transitions from one state to another $|n\rangle\langle m|$ are superpositions of degenerate excitations taken from all of the blocks $A^{(n)}$ with the corresponding parity. In contrast, the actual quasi-particle operators themselves (and combinations of them) are contained inside the blocks. While the introduction of an interacting term will break this block diagonal structure, see Figure 1, the above observation shows us that the many-body Majorana operators, which by definition are superpositions of odd-parity

$$\begin{aligned}
(a) \quad \mathcal{H}_Q &= \left[\begin{array}{l} \frac{\mu}{2} \sum_x \left[\begin{array}{c} \sigma^x \\ | \\ \sigma^y \end{array} \right] - \left[\begin{array}{c} \sigma^y \\ | \\ \sigma^x \end{array} \right] \\ \frac{t+\Delta}{2} \sum_x \left[\begin{array}{c} \sigma^x \\ / \\ \sigma^y \end{array} \right] - \left[\begin{array}{c} \sigma^y \\ / \\ \sigma^x \end{array} \right] \\ \frac{t-\Delta}{2} \sum_x \left[\begin{array}{c} \sigma^z \sigma^x \\ | \\ \sigma^y \sigma^z \end{array} \right] - \left[\begin{array}{c} \sigma^z \sigma^y \\ | \\ \sigma^x \sigma^z \end{array} \right] \end{array} \right] \\
(b) \quad \mathcal{H}_I &= \frac{U}{8} \sum_x \left[\begin{array}{c} \sigma^x \sigma^x \\ | \\ \sigma^y \sigma^y \end{array} \right] - \left[\begin{array}{c} \sigma^y \sigma^y \\ | \\ \sigma^x \sigma^x \end{array} \right] \\
(c) \quad \mathcal{N} - N I &= \sum_x \left[\begin{array}{c} \sigma^z \\ | \\ I \end{array} \right] - \left[\begin{array}{c} I \\ | \\ \sigma^z \end{array} \right]
\end{aligned}$$

FIG. 2. (a) Graphical representation of the block diagonal \mathcal{H}_Q . (b) Graphical representation of the quartic term \mathcal{H}_I . (c) The symmetry operator responsible excitation number conservation of \mathcal{H}_Q .

zero energy transitions, should be predominantly supported within the $A^{(1)}$ sector and therefore they are the odd-parity zero-energy modes that minimise their \mathcal{N} expectation values. This notion forms the basis for the algorithm that we define in the next section.

III. ALGORITHMS AND NUMERICS

A. Algorithms for computing zero-energy Majorana modes in the presence of local interactions

In Ref. 31 it was demonstrated that, in the $L \gg \xi$ limit, there was a well defined notion of the Majorana quasi-particle even in the presence of strong interactions. The stability of the Majorana to strong interactions follows from the fact that the degeneracy between all even-odd pairs remains to an order of perturbation theory that scales with the length of the system. Using the definition of Eq. 3 the position space many-body Majorana wave functions can then be calculated using the Trace (or Hilbert-Schmidt) inner-product. We have

$$\begin{aligned}
u_R^{(n)}(\vec{x}) &= \text{Tr}(\Gamma_x^{(n)} \times \gamma_R) / 2^N \equiv (\Gamma_x^{(n)} | \gamma_R) \quad (33) \\
u_L^{(n)}(\vec{x}) &= \text{Tr}(\Gamma_x^{(n)} \times \gamma_L) / 2^N \equiv (\Gamma_x^{(n)} | \gamma_L).
\end{aligned}$$

The full diagonalisation method (FD) is reviewed again in the Appendix D. Although very accurate, the algorithm is quite limited in the system sizes that it can handle. This is because, although the Hamiltonian is sparse, the eigenvectors are not, and we need all of them. In order to go to larger system sizes where we can probe systems with longer coherence

lengths we need another method. The approach we use is to focus on the Γ -representations of the commutator $\mathcal{H} = [H, \bullet]$. We call this procedure the commutator method (CM).

Like with the FD method, the key index in the CM algorithm is the number of position space sites N . The matrix representation scales as 2^{2N} where each $A^{(s)}$ block is spanned by $\binom{2N}{s}$ basis elements. In order to proceed we introduce physically motivated cut-offs for the number of basis elements that are needed to accurately represent the Majorana quasi-particle. The first cut-off N_s represents the maximum number of blocks $A^{(s)}$ that participate in the calculation. Thus an excitation number cut-off of $N_s = 3$ would only allow elements of $A^{(1)}$ and $A^{(3)}$, and a cut-off of $N_s = 9$ will only allow elements from blocks $A^{(1)}, A^{(3)}, A^{(5)}, A^{(7)}$ and $A^{(9)}$. The second cut-off is one where we only allow basis elements which can be reached by N_d operations of the Hamiltonian on full set of single-excitation basis elements that span $A^{(1)}$. This cut-off is in some ways similar to N_s but allows us to kick out basis elements used inside each of the $A^{(s)}$ sectors that are not in anyway close to the single-particle block. The algorithm is therefore in some way perturbative and therefore we do not expect it to be accurate at very high interactions. However, errors introduced can easily be controlled by demanding that results converge for sufficiently high cut-off values N_s and N_d .

While the cut-offs above allow us to fit the problem on a computer, another challenge is actually finding the particular zero-valued eigenstates of reduced operator \mathcal{H}_{red} which correspond to the Majorana quasiparticles. As we mentioned in the previous section the general method is to find the zero-valued solutions that minimise their expectation value of \mathcal{N} . While this is quite clear cut, there are serious convergence issues related to the fact that the particular zero-modes are sitting amongst many other zero and near-zero eigenstates of \mathcal{H}_{red} . We have found several robust methods which are in general agreement across a range of parameters.

The first and most straightforward method is to employ a Lanczos diagonalisation where the initial vector is chosen to be one of the two non-interacting modes. Using this method, with thin restarting, we can rapidly find the eigenstate with the correct properties, provided we have chosen N_s and N_d so that sufficient support is given to the many-particle structure of the mode. For small system sizes where it can be checked, the method gives results that are identical to that of the FD method, see Figure 3. We have also checked this procedure against two others. The first of these to evolve in imaginary time using sparse matrix recursive implementations of $\exp(-\mathcal{H}^2\tau)$ from an initial vector which is again one of the Majorana modes in the non-interacting regime. Given sufficiently large τ and high cut-offs off both N_s and N_d we typically see the convergence of eigenvalues to a value near zero and an expectation value for \mathcal{N} between 1 and 2. Recall that there are no other near-zero energy modes with this value of expectation value and therefore we know that if these two criteria are met that the results are an accurate representation of the true-many-body Majorana. The second method is to again use a Krylov subspace technique (in this case Arnoldi) to find as many near-zero eigenstates of \mathcal{H}_{red} as possible. We then

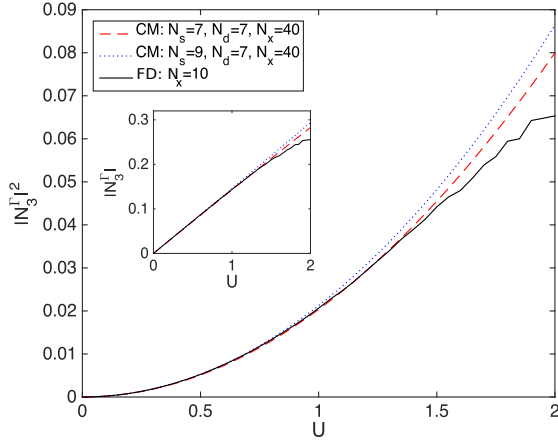


FIG. 3. In the figure we show the behaviour of $|N_3^\Gamma|^2$ for a system with $\Delta = 0.9$, $\mu = 1.5$ and $t = 1$. For $U = 0$ the Majorana mode has a coherence length of $\xi \approx 1.11$ and thus for small values of U permits us to use the full diagonalization method (FD) of Ref. 31. For this purpose we use a system size of $N_x = 10$. We compare this with results using the commutator method (CM) with $(N_s, N_d) = (7, 7)$ and $(7, 9)$ for a system of size $N_x = 40$. In the inset we plot the $|N_3^\Gamma|$ to emphasise the linear dependence on U .

search for the superposition of these states which minimises its expectation value of \mathcal{N} .

IV. NUMERICAL RESULTS

Our main numerical focus is on the N -particle participation ratios of the Majorana quasi-particle:

$$|N_n^\Gamma|^2 = \int |u_{L/R}^{(n)}(\vec{x})|^2 d\vec{x} \quad (34)$$

which have the property that $\sum |N_n^\Gamma|^2 = 1$. Our main findings, summed up in Figure 3 and Figure 4, are that

$$|N_3^\Gamma(U)| \propto \alpha_3 U \quad (35)$$

$$|N_5^\Gamma(U)| \propto \alpha_5 U^2 \quad (36)$$

$$|N_7^\Gamma(U)| \propto \alpha_7 U^3 \quad (37)$$

⋮

for odd values of n greater than 1. This linear U dependence shows that the 3-particle contributions to the many-body quasi-particle itself are therefore relevant even for small interactions strengths.

In Figures 5 and 6 we plot the dependence of the α_3 growth rate, which dictates how fast the higher 3-particle contributions to the Majorana quasi-particle grow as we increase the interaction strength U . We see from Figure 5 that there is a clear parabolic dependence centered around $\mu = 2t$. This value of the chemical potential corresponds to the half-filled band, where, in the lattice model, the energy-momentum dispersion is exactly linear. This shows that the growth of higher

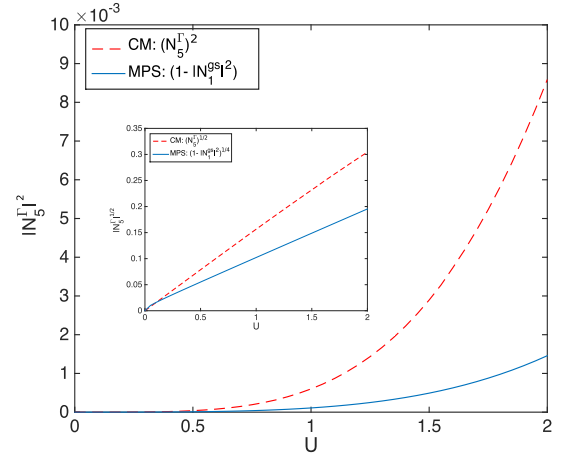


FIG. 4. In the figure we plot $|N_5^\Gamma(U)|^2$ and $1 - |N_1^{gs}(U)|^2$ for a system of $N = 40$ with $\Delta = 0.9$, $\mu = 1.5$ and $t = 1$. The inset shows that for these parameters $(1 - |N_1^{gs}(U)|^2)$ and $|N_5^\Gamma|^2$ grow as the 4th power of U . The quartic dependence of $1 - |N_1^{gs}(U)|^2$ would seem to indicate that single particle contributions should dominate even at higher interaction strengths (Note the small scale on the Y-axis of the main figure). However, as we discuss in section V the linear correlators are not a reliable indicator of the N -particle content of the quasi-particle itself. Indeed we note that the $|N_5^\Gamma|^2$ shown here is far smaller than $|N_3^\Gamma|^2$ shown in Figure 3 for the same system parameters.

N contributions is sensitive to the precise nature of the underlying dispersion. Figure 6 also shows the clear reduction of the α_3 growth rate as the superconducting gap is made larger. The same general trends are also seen for the $\alpha_5^{1/2}$ parameter, see appendix E.

In Figure 4 we also compare an example $|N_5^\Gamma|^2$ with the measure $1 - |N_{gs}|^2$ where

$$|N_{gs}|^2 = \int |O_{L/R}^{gs}(x)|^2 dx \quad (38)$$

and where O is the single-particle operator expansion of the ground state outerproducts such that

$$\begin{aligned} |O_{R/L}(x)| &= |\langle 0_e | c_x^\dagger \pm c_x | 0_o \rangle| \\ &= |\text{Tr}(c_x^\dagger \pm c_x \times |0_o\rangle\langle 0_e|)| \end{aligned} \quad (39)$$

To calculate the ground state correlators we use a customised MPS algorithm similar to that outlined in⁴¹. In general agreement with Ref. 24, which calculated the same measure for the related proximity coupled model, we see that $|N_{gs}|$ tends to stay very close to unity even at higher interaction strengths. On the surface this would seem to imply a much lower multi-particle contributions than that predicted using the FD and CM methods above. In section V we show that while $|O^{gs}(x)|$ is a valuable measure for understanding the general position space spread of the Majorana operators, it is not a reliable indicator of the N -particle participation rates in the quasi-particles themselves.

Before moving on we note that the trace expression in Eq.

V. MEASURING THE MANY-BODY MAJORANA STRUCTURE WITH DMRG AND MPS

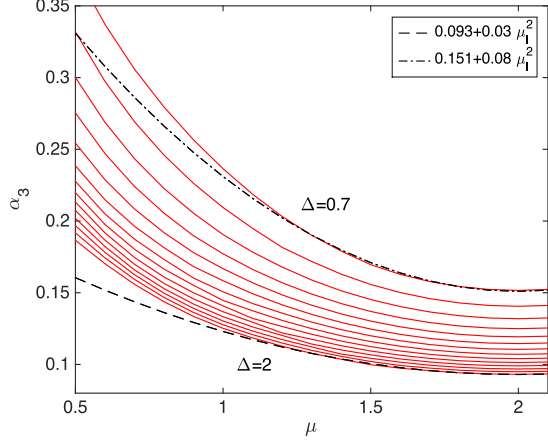


FIG. 5. In the figure we plot α_3 , the rate of slope of the $|N_3^\Gamma(U)|$ as a function of μ . Our results show best convergence for small coherence lengths and values of the μ that are far from the bottom of the band. We see a clear quadratic dependence centered around $\mu = 2t$. Thus the rate of growth of this term is least when we can linearise our dispersion (at $\mu = 2$). Fits of quadratic curves that show good overlap with the numerical data are also given. A system size of $N_x = 50$, with cutoffs $(N_s, N_d) = (9, 9)$ was used for this plot.

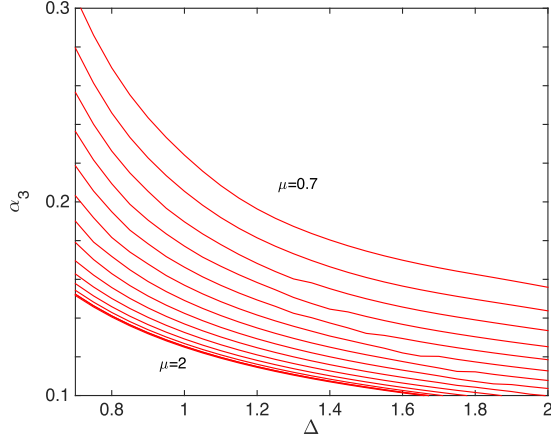


FIG. 6. In the figure we plot the rate α_3 as a function of Δ . The rate of growth clearly increases as Δ decreases. The N-particle content of the many-body Majorana is therefore clearly grows with the increased coherence length associated with a smaller superconducting gap. A system size of $N_x = 50$, with cutoffs $(N_s, N_d) = (9, 9)$ was used for this plot.

(39) does not contain the same factor $1/2^N$ as the expressions in Eq. (33). Then (39) actually represents the single particle operator expansion of the ground-state outer product $|0_o\rangle\langle 0_e|$ that has been multiplied by a factor of 2^N . We will see in the next section, that only in the case of a non-interacting system does this magnified single-particle expansion correspond to the structure of the quasi-particle.

When the interactions are included, the linear form (1) is no longer sufficient to fully describe the Majorana zero-mode. The operators, which are Hermitian, particle-hole symmetric and have odd parity (i.e. it switches the parity of the underlying states) can be expanded in multinomials of terms with odd fermionic parity, see Eq. 2.

The Majorana operator takes us from one ground state to the other $|\langle 0_e | \gamma_{L/R} | 0_o \rangle| = 1$. For the non-interacting system one way to read-off the full Majorana operator structure is to examine the correlations $\langle 0 | \Gamma_a^{(1)} | 0 \rangle_o$ where the ground states $|0\rangle_{e/o}$ are obtained from variational techniques such as DMRG or MPS, and the Γ_a operators are restricted to the $2N$ single particle operators γ_i . In the non-interacting limit the values obtained from analysis of these single-particle cross-correlators are enough to fully determine the structure of the Majorana operator where the calculation on the left hand side of the system, is as follows:

$$\begin{aligned} O_L(x') &= \langle 0_e | \Gamma_{x'}^{(m)} | 0_o \rangle = \langle 0_e | m_{x'} \gamma_L | 0_o \rangle \\ &= \sum_x u_L(x) \langle 0_e | m_{x'} m_x | 0_e \rangle = u_L(x') \end{aligned}$$

The last equality follows because, for arbitrary normalised states $|\psi\rangle$, $m_{x_1}|\psi\rangle$ and $m_{x_2}|\psi\rangle$ are orthonormal (i.e. $\langle \psi | m_{x_1} m_{x_2} | \psi \rangle = \delta_{x_1, x_2}$ see below). The calculation shows that, by examining the cross-correlators $\langle 0_e | \Gamma_{x'}^{(1)} | 0_o \rangle$ we can learn the form of the non-interacting Majorana operators. Of course this approach is not really necessary for the non-interacting system, as we can also work out the free fermion excitations from the single transition BdG/Majorana representations.

It is often assumed that because this method works in the non-interacting regime, it should work equally well in the presence of interactions. As we now show, this assumption is wrong, and the cross-correlations cannot be used to resolve the precise form of the many-body Majorana (2). We can understand this on a basic level by just noting that the ground-state outer-products are not the same as the Majorana expansions formed using all the eigenstates of the system, see Ref. 31. However, it is also illustrative to observe where the simple calculation presented above breaks down when interactions are present. We will see that in this case, because the Majorana operators will now contain contributions from operators like $\Gamma_x^{(3)}$, $\Gamma_x^{(5)}$, etc. (see Eq. (2)), and because a more complicated set of orthonogonality relations exist between generic states $\Gamma_x^{(n)}|\psi\rangle$ and $\Gamma_{x'}^{(m)}|\psi\rangle$, that

$$\langle 0_e | \Gamma_x^{(n)} | 0_o \rangle \neq u^{(n)}(x). \quad (40)$$

To see these general orthonormal conditions lets suppose we have an operator W that has been constructed from two odd-number sequences of γ operators $W = \Gamma^{(l)}\Gamma^{(m)}$. Now consider when, for arbitrary real states $|\psi\rangle$, does the correlation $\langle \psi | W | \psi \rangle$ vanish. The constituent operators γ are uni-

tary operators and they therefore take any position space *basis* element to an orthogonal basis element with opposite occupancy on the sites where the operator W has acted: $\langle n_x | n'_x \rangle = \langle n_x | W | n_x \rangle = 0$. Here the n_x are binary number sequences indicating the occupancy on each position space site.

As the p-wave Hamiltonian can always be made real,² all eigenstates are also real. For any operator W we can therefore always decompose any eigenstate $|\psi\rangle$ as

$$|\psi\rangle = \sum_n (a_n + \phi b_n W |n\rangle) \quad (41)$$

where the sum is over half of the basis elements. Here we also assume both a_n and b_n are real but an extra phase $\phi = i^{N_m}$, that depends on the precise number of m -type γ 's in W , is also included before the b_n .

Now lets consider the correlator

$$\begin{aligned} \langle \psi | W | \psi \rangle &= \sum_{nm} \langle m | (a_m + \phi^* b_m W^\dagger) W (a_n + \phi b_n W) | n \rangle \\ &= \sum_n a_n b_n (I \pm I) \end{aligned} \quad (42)$$

with the \pm depending on whether $(\phi W)^2 = \pm I$.

In the cases where $(\phi W)^2 = -I$ the correlator vanishes. To see when this occurs we need to consider (1) how many permutations or swaps are needed to bring all operators in two identical words (each of length N_w) together and (2) how many different m -type terms occur. As one needs precisely $N_w(N_w + 1)/2$ single swaps to bring all corresponding operators in W^2 together and N_m is the number of m 's in a word (and N_p is the number of p 's such that $N_m + N_p = N_w$) we see the general condition for the correlators to vanish is that $N_v = N_w(N_w + 1)/2 + N_m$ is odd.

For the case analysed above where we have $W = m_x m'_x$, we see that $N_w = 2$ and $N_m = 2$ and therefore $N_v = 5$. Clearly then $m_x |\psi\rangle$ and $m'_x |\psi\rangle$ are orthogonal for an arbitrary real state $|\psi\rangle$. Although it is not generally true that $p_x |\psi\rangle$ and $m'_x |\psi\rangle$ are orthogonal, because the relevant p_x and m_x operators tend to be on opposite sides of the system, this does not necessarily present a problem. However, if we consider for example terms such as $p_{x_1} m_{x_2} m_{x_3}$, we see that these types of correlations are tend to localise to the same side of the system as m_x . Furthermore we see from the considerations above, that the overlap between states $p_{x_1} m_{x_2} m_{x_3} |\psi\rangle$ and $m_x |\psi\rangle$ only vanishes only when x is not equal to x_2 or x_3 . This means that in the interacting system, any measure of the single-particle cross-correlators $\langle 0_e | m_x | 0_o \rangle$ is not independent from contributions from the multi-particle part the Majorana operator. In appendix F, we discuss the possibility of using a sub-sets of operators to represent the mapping between ground states, placing an emphasis on sets of operators that produce states that are almost orthogonal to each other.

VI. CONCLUSION

In this paper we have examined the Majorana zero-energy quasi-particles in an interacting regime. We have used the fact

that the commutator of the free-system can, in the matrix representation generated by Majorana operators, be written in a block-diagonal form such that free-particles are the eigen-solutions of the sub-block encoding single particle excitations. We showed that interactions will disrupt this block diagonal structure and force eigen-operators to be superpositions of operators from other sub-blocks encoding multiply-particle transitions. However in the case of Majorana zero-modes in an interacting regime, because the interactions fails to lift degeneracies, we can superpose these zero-energy transitions such that the resulting operator is contained mostly in one of these sub-blocks. The many-body Majorana quasi-particle can be thought of as the particular superposition of zero-energy odd-parity transitions that minimise the excitation number.

We used this idea to calculate the multi-particle content of the Majorana zero modes in the presence of interactions. Our main observation is that in the presence of interactions the multi-particle content of these Majorana excitations can be significant. In retrospect this is to be expected because in the definition of the mode we use all energy eigenstates, and interactions should easily generate mixing between eigenstates of the same parity that are not separated by an energy gap. At first sight this may conflict with our intuitive understanding of what a topological phase should be. However, as we already noted, in the non-interacting regime the *structure* of Majorana mode is also very sensitive to small changes of the system parameters and indeed, in it can be argued that this fluidity is the reason the topological degeneracy is so stable.

A significant portion of the paper has dealt with the issue of the ground state correlators and how they are related to the Majorana modes in the presence of interactions. We have pointed out that these correlators cannot be used to reliably infer the multi-particle content of the zero-modes. On this point, it is legitimate to ask how important is the strong quasi-particle picture anyway? After all, the experimentally relevant physical quantities *will* be dominated by the properties of the low energy states alone, and we expect that the multi-particle content of the mode will only have an oblique relationship with actual experimental data. However, this indirect association *does* have important implications for how we should interpret experimental data and in particular implies that we should not be too quick to associate experimental data with the single-particle content of the mode itself.

VII. ACKNOWLEDGEMENTS

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Appendix A: A brief review of the 1d p-wave lattice model

We are concerned generally with situations where our system can be written as a sum of $H = H_Q + H_I$ where H_Q is quadratic free-fermion Hamiltonian

$$H_Q = \frac{1}{2} \sum_{i,j=1}^N A_{ij}^{(1)} \gamma_i \gamma_j \quad (\text{A1})$$

for imaginary A_{ij} and the interacting terms is a quartic term of the form

$$H_I = \sum_{ijkl} v_{ijkl} \gamma_i \gamma_j \gamma_k \gamma_l \quad (\text{A2})$$

where i, j, k and l are from the same local neighbourhood. The constituent components of here are the position space Majorana terms defined in term of complex Dirac Fermion operators c^\dagger and c :

$$\begin{aligned} p_n &= \gamma_{2n-1} = (c_n^\dagger + c_n) \\ m_n &= \gamma_{2n} = i(c_n^\dagger - c_n) \end{aligned} \quad (\text{A3})$$

which obey $\{\gamma_i, \gamma_j\} = 2\delta_{ij}$ and thus $\gamma_i = \gamma_i^\dagger$ and $\gamma_i^2 = I$.

In the main text the particular quadratic model that we have in mind is the 1d spin-less p-wave superconducting model²

$$\begin{aligned} H_Q &= \frac{i}{2} \sum_j^N \mu p_j m_j + \frac{i}{2} \sum_{j=1}^{N-1} (|\Delta| + t) m_j p_{j+1} \\ &+ \frac{i}{2} \sum_{j=1}^{N-1} (|\Delta| - t) p_j m_{j+1} \end{aligned} \quad (\text{A4})$$

where we have without loss of generality chosen the phase of the p-wave superconducting pairing potential to be real. The quartic term we use is of the form

$$H_I = \frac{U}{8} \sum_j p_j m_j m_{j+1} p_{j+1} \quad (\text{A5})$$

When $|\Delta| > 0$ and $|\mu| < 2t$ the H_Q system is known to be in a topological phase with a Majorana zero modes exponentially localized at each end of the wire². We will typically work with $\mu = \mu_l + 2t$ so that we identify $\mu = 0$ as the bottom of the band and the starting point of the topological phase. The transverse Ising model corresponds to the special case of this

model where $U = 0$ and $t = \Delta$.

Appendix B: A spin representation for the Γ basis

The matrix \mathcal{H} scales as $4^N \times 4^N$. For $N > 8$ this becomes something that is difficult to store on a computer, even if sparse matrix technology is employed. Ideally we would like to be able to represent this matrix in a more abstract fashion as a sum over operators, in analogy with the way we generate the usual Hamiltonian with a sum over operators that act on basis states in a well defined way.

We will show how to build our Hilbert space using the $\left| \Gamma_a \right\rangle$ eigenbasis and the $\left| \Sigma \right\rangle$ basis. One of the nice things about the γ operators in general is that they are non-projective, we therefore have on a single site

$$m_n I = m_n \quad (\text{B1})$$

$$p_n I = p_n \quad (\text{B2})$$

$$p_n p_n = m_n m_n = I \quad (\text{B3})$$

$$iZ_n = m_n p_n \quad (\text{B4})$$

$$m_n (iZ_n) = p_n \quad (\text{B5})$$

$$p_n (iZ_n) = -m_n \quad (\text{B6})$$

which means that when acting to the right on a basis defined by

$$\left| I \right\rangle = \left| 00 \right\rangle = [1, 0]^T \otimes [1, 0]^T = [1, 0, 0, 0]^T, \quad (\text{B7})$$

$$\left| p \right\rangle = \left| 01 \right\rangle = [1, 0]^T \otimes [0, 1]^T = [0, 1, 0, 0]^T,$$

$$\left| m \right\rangle = \left| 10 \right\rangle = [0, 1]^T \otimes [1, 0]^T = [0, 0, 1, 0]^T,$$

$$\left| iZ \right\rangle = \left| 11 \right\rangle = [0, 1]^T \otimes [0, 1]^T = [0, 0, 0, 1]^T$$

we have

$$\bar{p}^R = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{bmatrix} = \sigma^z \otimes \sigma^x \quad (\text{B8})$$

$$\bar{m}^R = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} = \sigma^x \otimes I_2 \quad (\text{B9})$$

To enforce anti-commutation relations between different sites we need to attach Jordan-Wigner (JW) like strings which should anti-commute with m^R and p^R but take all basis elements onto themselves. In the above basis, one such operator is

$$S = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \sigma^z \otimes \sigma^z. \quad (\text{B10})$$

and we then have

$$m_x^R = \left[\prod_{j=1}^{x-1} S_j \right] \times \bar{m}_x^R, \quad p_x^R = \left[\prod_{j=1}^{x-1} S_j \right] \times \bar{p}_x^R \quad (\text{B11})$$

$$(\text{B12})$$

Similarly for the action to the left can write have

$$\bar{p}^L = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = I_2 \otimes \sigma^x \quad (\text{B13})$$

$$\bar{m}^L = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} = \sigma^x \otimes \sigma^z \quad (\text{B14})$$

In order to enforce anti-symmetry of the left-acting operators alone we can choose our JW-strings so that they come from the opposite direction

$$m_x^L = \left[\prod_{j=x+1}^{N_x} S_j \right] \times \bar{m}_x^L, \quad p_x^L = \left[\prod_{j=x+1}^{N_x} S_j \right] \times \bar{p}_x^L$$

However, this choice means that operators from the left and right commute. This does not have to be the case and we can also choose our J-W strings so that all operators anti-commute. One such choice would be to set

$$m_x^R = \left[\prod_{j=1}^{x-1} S_j \right] \times \bar{m}_x^R, \quad p_x^R = \left[\prod_{j=1}^{x-1} S_j \right] \times \bar{p}_x^R$$

and

$$m_x^L = i \left[\prod_{j=1}^x S_j \right] \times \bar{m}_x^L, \quad p_x^L = -i \left[\prod_{j=1}^x S_j \right] \times \bar{p}_x^L$$

where the additional i phases are chosen so that $m^2 = p^2 = I$. Note that there is some freedom in the choice of overall sign here which can be useful for switching the overall sign of H_L for example.

Appendix C: A spin basis for Dirac fermions

In the previous section we showed how to build up a representation for the $\left| \Gamma \right\rangle$ basis which is based on the properties of the Clifford algebra. However there are other ways to do this. Consider the Fock space representation for a single two level

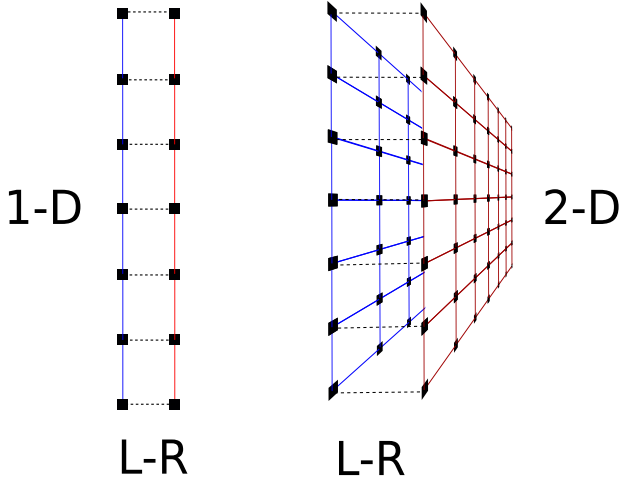


FIG. 7. Fermionic doubling: in the Σ -basis the commutator $[H, \bullet]$ can be understood as two disconnected copies of original system.

mode we have

$$\begin{aligned}
\sigma^+ &= +|1\rangle\langle 0| \\
\sigma^- &= +|0\rangle\langle 1| \\
\sigma^- \sigma^+ &= +|0\rangle\langle 0| \\
\sigma^+ \sigma^- &= +|1\rangle\langle 1| \\
\sigma^- \sigma^+ + \sigma^+ \sigma^- &= I_2 = +|0\rangle\langle 0| + |1\rangle\langle 1| \\
\sigma^z &= -|0\rangle\langle 0| + |1\rangle\langle 1|
\end{aligned} \tag{C1}$$

Now for a single site we choose

$$(\Sigma^1 \downarrow) = (\sigma^- \sigma^+ \downarrow) = [1, 0, 0, 0] \tag{C2}$$

$$(\Sigma^2 \downarrow) = (\sigma^+ \downarrow) = [0, 1, 0, 0] \tag{C3}$$

$$(\Sigma^3 \downarrow) = (\sigma^- \downarrow) = [0, 0, 1, 0] \tag{C4}$$

$$(\Sigma^4 \downarrow) = (\sigma^+ \sigma^- \downarrow) = [0, 0, 0, 1] \tag{C5}$$

To represent each operator in this basis we need to see how the operators act to both the right (on $\downarrow \Sigma$) states) and the left (on $\downarrow \Sigma$ states). As will be see, it is enough to examine just σ^- in each scenario. Acting to the right the σ^- operator should send $\downarrow \sigma^+ \sigma^- \rightarrow \downarrow \sigma^-$ and $\downarrow \sigma^+ \rightarrow \downarrow \sigma^- \sigma^+$. Therefore we have

$$\sigma_R^- = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{C6}$$

On the other hand, when acting to the left, σ^- should send $(\sigma^+ \sigma^- \downarrow) \rightarrow (\sigma^+ \downarrow)$ and $(\sigma^- \downarrow) \rightarrow (\sigma^- \sigma^+ \downarrow)$. Recall that when operating to the left, the conjugate of the operating term appears inside the left-hand-side basis state, but to the right of

the existing operator label. Therefore we write

$$\sigma_L^- = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \tag{C7}$$

The importance of this particular basis becomes clear when we examine the \pm superposition and we have

$$X^R = \sigma_R^+ + \sigma_R^- = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = I \otimes \sigma^x$$

$$X^L = \sigma_L^+ + \sigma_L^- = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} = \sigma_x \otimes I$$

$$Y^R = i(\sigma_R^+ - \sigma_R^-) = \begin{bmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{bmatrix} = I \otimes \sigma^y$$

$$Y^L = i(\sigma_L^+ - \sigma_L^-) = \begin{bmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \\ -i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{bmatrix} = -\sigma_y \otimes I$$

To create a fermionic basis we can attach Jordan-Wigner strings and we could write for example the Majorana fermion operators as

$$p_n^R = I \otimes (c_n^\dagger + c_n) = \left[\prod_{i=1}^{n-1} I \otimes \sigma_i^z \right] X_n^R \tag{C8}$$

or

$$m_n^L = i(c_n^\dagger - c_n) \otimes I = \left[\prod_{i=1}^{n-1} \sigma_i^z \otimes I \right] Y_n^L \tag{C9}$$

The $\downarrow \Sigma$ representation above reveals that left operating operators act on an entirely different sub-space to the right. This means that we can represent any transition Hamiltonian matrix as

$$\mathcal{H} = [H, \bullet] = I \otimes H - H \otimes I = H_R - H_L \tag{C10}$$

and therefore the transition matrix is simply a trivial doubling of the original Hamiltonian but where all constants on one Hamiltonian have been negated. Similar observations with respect to integrability have been made in the context of parafermions.³⁴ For a 1-d and 2-d systems this lends itself to the easy visualisation shown in Figure 7.

We are free to interpret the transition Hamiltonian [1] as separate fermionic systems but where the fermions of left and

right do not anti-commute with each other or [2] as single fermionic system which simply happens to have no terms than connect the sites with index L to any sites with index R . This can easily be achieved in the construction above by choosing a Jordan-Wigner string convention that runs through both indices L and R . In this latter picture the opposite overall sign on the H_L terms can make interpretation slightly more cumbersome, in particular for lattice system where we would like to take the continuum limit. However, we note that the trivial transformation $c_L^\dagger \leftrightarrow c_L$ sends $m_L \rightarrow -m_L$ and therefore any left-hand terms with an odd number of m -type operators will also change sign under this change of basis.

This $|\Sigma\rangle$ basis is related to the $|\Gamma\rangle$ basis by Hadamard rotations from the p and m to the c^\dagger and c together with additional Hadamard rotations from Z and I to the $c^\dagger c$ and $c c^\dagger$. The first transformation is what we understand on the single particle level as a change of basis from a Bogoliubov deGennes representation to a Kastelyn-like Majorana adjacency representation. These rotations take place entirely within each of the sub-blocks $A^{(n)}$. By contrast, the second transformation mixes between different $A^{(n)}$ sub-blocks. In section II C we show that this transformation is essential to understanding relationship between solutions of each sub-block and actual eigensolutions of the full commutator $|n\rangle\langle m|$.

Appendix D: Review of full-diagonalization method (FM) for computing zero-energy Majorana modes in the presence of local interactions

In Ref. 31 it was demonstrated that, in the $L \gg \xi$ limit, there was a well defined notion of the Majorana quasi-particle even in the presence of strong interactions. The stability of the Majorana to strong interactions follows from the fact that the degeneracy between all even-odd pairs remains to an order of perturbation theory that scales with the length of the system. This degeneracy then allows one to calculate the precise structure of the Majorana modes by:

- (1) Calculating all eigenfunctions of even and odd sectors.
- (2) Identifying even-odd counterparts by checking for example that $\langle n_o | \gamma_L(U=0) | n_e \rangle$ is close of the order of unity.
- (3) Fixing the relative phases of all even-odd pairs using the bare-non interacting Majorana modes. For the situation with real coefficients only we calculate $s_n^{(R)} = \text{sign}(\langle n_o | \beta_1^\dagger + \beta_1 | n_e \rangle)$ and set $|n_o\rangle \rightarrow s_n^{(R)} |n_o\rangle$.
- (4) Finally with $s_n^{(L)} = \text{sign}(\langle n_o | \beta_1^\dagger - \beta_1 | n_e \rangle)$, we can then write

$$\begin{aligned} \gamma_R &= \sum I |n_o\rangle\langle n_e| + I |n_e\rangle\langle n_o| \quad (\text{D1}) \\ \gamma_L &= i \sum s_n^{(L)} |n_o\rangle\langle n_e| - s_n^{(L)} |n_e\rangle\langle n_o|. \end{aligned}$$

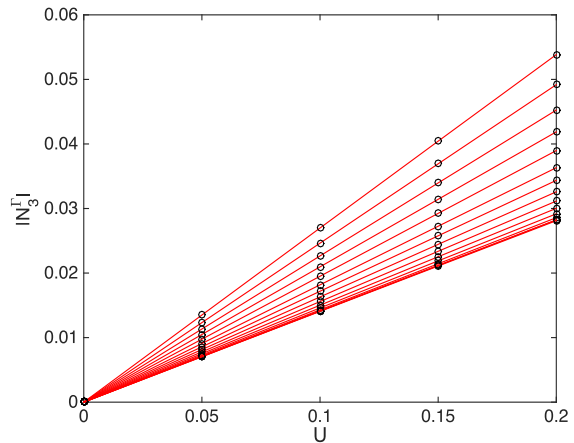


FIG. 8. In the figure we show how $|N_3^\Gamma|$ grows for a fixed value of $\Delta = 0.8$ and different values of $\mu \in [0.7, 2.1]$. The values of α_3 at different parameters represent the slopes of these straight lines. A system size of $N_x = 50$, with cutoffs $(N_s, N_d) = (9, 9)$ was used for this plot.

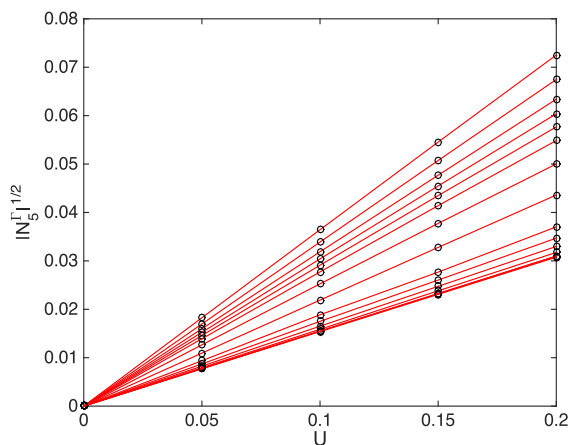


FIG. 9. In the figure we show how $|N_5^\Gamma|^{1/2}$ grows for a fixed value of $\Delta = 0.7$ and different values of $\mu \in [0.7, 2.1]$. The values of $\alpha_5^{1/2}$ at different parameters represent the slopes of these straight lines. A system size of $N_x = 50$, with cutoffs $(N_s, N_d) = (9, 9)$ was used for this plot.

Appendix E: Additional Numerical results

In this section we provide additional numerics which give further support for the central claims of the main text regarding the N-particle content of the Majorana zero modes. In Figure 8 we clearly see how $|N_3^\Gamma|$ depends linearly on U for a variety of system parameters. A similar story is also evident in Figure 9 where we plot $|N_5^\Gamma|^{1/2}$ for a variety of system parameters. Although the linear dependence on U is clear we see some apparent fluctuations in how the slope changes for different values of μ .

We plot the values of $\alpha_5^{1/2}$ directly in Figures 10 and 11.

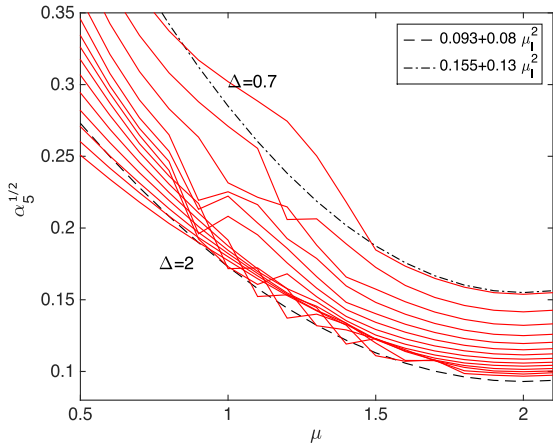


FIG. 10. In the figure we plot the rate $\alpha_5^{1/2}$ as a function of μ . We again see a quadratic dependence about the linearised dispersion point at $\mu = 2$. The plot shows some numerical instability. Note that to fit these curves we take the $|N_5|^{1/4}$ and very small numerical errors get magnified to some degree. A system size of $N_x = 50$, with cutoffs $(N_s, N_d) = (9, 9)$ was used for this plot.

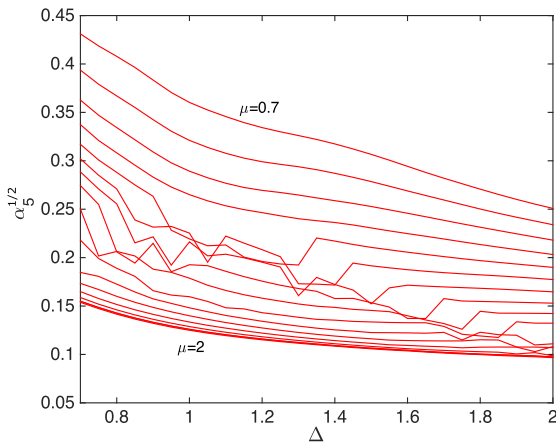


FIG. 11. In the figure we plot the rate $\alpha_5^{1/2}$ as a function of Δ . A system size of $N_x = 50$, with cutoffs $(N_s, N_d) = (9, 9)$ was used for this plot.

We note that $\alpha_5^{1/2}$ has the same general dependence on μ and Δ as α_3 . However we also see that the fluctuations in $\alpha_5^{1/2}$ are not specific to the parameters used for Figure 9 above. We suspect that the fluctuations are probably a numerical artefact resulting from the finite cut-offs mentioned in section III. Nonetheless, since we have not been able to remove this effect by going to larger system sizes (and larger cut-offs) we cannot discount the possibility that it is due to some unknown physical effect.

Appendix F: Complete operator sets for mapping between ground states

In section V we argued that ground state correlation data cannot be used to infer the structure of the Majorana mode in

the interacting regime. This is because the problem of finding an operator such that $|\langle 0_e | O | 0_o \rangle| = 1$ is underdefined, and there are many different ways of satisfying this criteria. Nonetheless, it is still meaningful to try to find a sensible expansion (in position space operators Γ_a) of an operator O that fits the aforementioned criteria.

Ideally we would like to find a sets of 2^{N-1} operators that send some arbitrary state $|\psi\rangle$ (i.e one of the ground states) to an orthonormal basis of states in the other sector. This would allow us to uniquely capture the structure of the two Majorana zero-mode operators which connect ground states in even(odd) sectors. We find that it is relatively easy to find a set of operators that gives an independent basis. Orthogonality on the other hand, while achievable, requires one to employ a procedure such as Gram-Schmidt and the resulting operators end up being complicated superpositions which do not allow us to extract any physical intuition.

Although orthogonality is not practical, it is possible to come up with a set of operators that generate a partially orthonormal basis. This then does allow us some intuitive understanding of the Majorana zero-mode structure in the sense implied by Ref. 24. This operator choice for the p-wave system is outlined in Table I. An appealing property of this choice is that the *ppp*-type operators are always ‘orthogonal’ to *m*-type in the sense that for any state $|\psi\rangle$ we have $\langle \psi | m_{x_1} p_{x_2} p_{x_3} p_{x_4} | \psi \rangle = 0$. Indeed, each sub-set of operators picks out states that are always orthogonal to the states picked out by the set immediately above or below them in the table. The problem arises however in that, apart from the single particle rows $\Gamma^{(1)}$, each set of operators is not orthogonal with elements of the same type when these operators overlap on one common site, see section V. By the same reasoning, members of the set *mmmm* overlap with members of *m*, and states obtained by operating with *ppp* will have to overlap with some members of *pppppp* etc. Therefore, even with this carefully chosen set of operators, the condition $|\langle 0_e | O | 0_o \rangle| = 1$ does not appear to be restrictive enough to define a unique operator.

	Left-localised	Right-localised
$\Gamma^{(1)}$	<i>m</i>	<i>p</i>
$\Gamma^{(3)}$	<i>p p p</i>	<i>mmm</i>
$\Gamma^{(5)}$	<i>mmmmm</i>	<i>p p p p p</i>
$\Gamma^{(7)}$	<i>p p p p p p p</i>	<i>mmmmmmm</i>
	\vdots	\vdots

TABLE I. A set of $2n - 1$ point correlators that can be used to describe the many-body Majorana operators. In the table the *m* stands for m_x , *ppp* stands for $p_{x_1} p_{x_2} p_{x_3}$ etc. where $m_x = i(c_x^\dagger - c_x)$ and $p_x = c_x^\dagger + c_x$.