Probing Majorana modes in the tunneling spectra of a resonant level

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Abstract

Unambiguous identification of Majorana physics presents an outstanding problem whose solution could render topological quantum computing feasible. We develop a numerical approach to treat finite-size superconducting chains supporting Majorana modes, which is based on iterative application of a two-site Bogoliubov transformation. We demonstrate the applicability of the method by studying a resonant level attached to the superconductor subject to external perturbations. In the topological phase, we show that the spectrum of a single resonant level allows us to distinguish peaks coming from Majorana physics from the Kondo resonance.

(Some figures may appear in colour only in the online journal)

1. Introduction

Condensed matter theory, in the course of its continued quiet revolution, has endowed our understanding of nature by introducing quasiparticles with diverse, often exotic, behavior. A prominent example is a Majorana mode. The Majorana fermion was originally introduced in the context of particle physics [1] as a particle being its own antiparticle. The possibility of having Majorana fermion-like quasiparticles, Majorana modes, in a solid state system, has attracted a lot of attention, because of their potential for quantum computing. Information carried this way would be essentially non-local and retrieved by certain non-Abelian operations (braiding), being rather immune to general disturbances of the environment [2–5]. Although several condensed matter environments could support Majorana modes [6–10], topological superconductors [11–13] have emerged as a natural playground. The latter are not restricted to rare materials, rather they are engineered easily by forming appropriate heterostructures with ordinary s-wave superconductors [14, 15]. Experimental setups, which, based on predictions, could host Majorana modes, have been prepared [16–19], but their unambiguous experimental observation is a task far from being obvious. A very promising route is offered by transport measurements, since Majorana modes should give rise to a zero-bias resonance which does not react to weak changes of magnetic field or gate voltage. However, conductivity enhancement near zero bias is a common companion of diverse collective phenomena. Examples are Kondo effect, 0.7 anomaly [20, 21], Tamm–Shockley bound states at the end of a charge-density wave wire [22–24], or the recently proposed electronic disorder [25]. Thus, a careful elimination of these scenarios should be a part of the ‘smoking-gun’ probe of the Majorana mode. We would like to contribute to this debate by studying a superconducting system whose local spectral function exhibits resonances coming from two sources: the topologically protected Majorana mode and a single-particle electronic resonance.

Our model system consists of a single level weakly coupled to a one-dimensional superconductor. We consider both singlet and triplet pairing mechanisms. We firstly verify that the resonance of the single level survives after coupling to a singlet-paired superconductor. We observe that the position of the resulting resonance is coupled to the external gate voltage. When singlet pairing is replaced by the triplet one, the superconductor model is the well known Kitaev chain [12] doubled due to spin degeneracy, having Majorana states at both ends of the chain\textsuperscript{3}. These modes give rise to resonances

\textsuperscript{3} Per spin, there is a single fermionic boundary mode, which corresponds to two separate Majorana states.
in the local spectrum at zero energy. The nature of the coupling of one of the Majorana states to the resonant level (RL) is revealed in the behavior of the resonances upon local gating and weak magnetic field. Among the plethora of peaks, the RL manifests itself due to the coupling to the external fields, in contrast to the Majorana peak. Thus, the distinctive behavior of the peak structure allows us to suggest a new means of experimental demonstration of Majorana physics.

In order to see the behavior of the resonances, it is sufficient to look at local spectral functions, which directly convey the electron/hole tunneling spectral density. The calculation of spectra involves solving for the eigenstates of the Hamiltonian with superconducting mean-field terms, i.e. a general Hermitian operator which is bilinear in fermionic operators. To this end, we have developed a numerical method which preserves canonical anti-commutation rules. We employ a numerical diagonalization based on iterative application of Bogoliubov transformation [26] to a Fock subspace spanned by two orbitals. This is an extension of the Jacobi diagonalization procedure: we not only consider basis changes, but also general automorphisms of the Fermi operator algebra.

From a theoretical standpoint, this approach relies on a fully fermionic language. Thus, it is capable of providing intuitively transparent arguments, like occupation numbers, with superconducting mean-field terms, i.e. a general Hamiltonian is written in a matrix form

\[
H = \sum_{x} \Psi_{x} H \Psi_{x}^\dagger \text{ (see appendix C) with the matrix } H \text{ of the form}
\]

\[
H = \begin{pmatrix} \frac{1}{2}h & b \\ b^\ast & -\frac{1}{2}h^\ast \end{pmatrix}.
\]

Diagonalization of \( H \) leads to the spectrum, but does not guarantee fermionic anti-commutation relations. Note that due to the particle–hole transformation of the down spin fermions the diagonal part of \( h \) might be changed. Therefore we denote it with \( \tilde{h} \). If the diagonal form is achieved by the unitary matrix \( U \), the transformation need not be canonical. Because the eigenvalues of \( H \) come in pairs \( \pm \epsilon \), the matrix \( U \) contains correct eigenvectors if no degeneracies are present, but not in a general case. We note that canonical relations are not guaranteed in the Green’s function approach [30] for the same reason as outlined above.

Since we wish to treat a general class of systems with arbitrary degeneracies, we present a method which explicitly preserves canonical commutation rules. This is a crucial step for the calculation of local spectral functions. Before we explain the full procedure, we illustrate a few important points in the two-orbital case.

2.2.1. Dimer

We start with a simple two-orbital (dimer) Hamiltonian described by

\[
H = \epsilon \hat{c}_{1}^\dagger \hat{c}_{1} + \epsilon' \hat{c}_{2}^\dagger \hat{c}_{2} + t(\hat{c}_{1}^\dagger \hat{c}_{2} + \hat{c}_{2}^\dagger \hat{c}_{1}) + \Delta(\hat{c}_{2}^\dagger \hat{c}_{1} + \hat{c}_{1}^\dagger \hat{c}_{2})
\]

with two unequal on-site terms, a hopping term and the superconducting pairing term. For convenience, the Hamiltonian is written in a matrix form

\[
H = \begin{pmatrix} \epsilon & t & \Delta \frac{1}{2} \\ t & \epsilon' & -\Delta \frac{1}{2} \\ \Delta \frac{1}{2} & 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{c}_{1} \\ \hat{c}_{2} \\ \hat{c}_{1}^\dagger \end{pmatrix}.
\]
where the row and column vectors are similar to Nambu spinors, see appendix C. We bring it to a diagonal form in a two-step procedure. Firstly, we transform away the anomalous pairing terms by a Bogoliubov transformation. Then the Hamiltonian attains a coupled two-level structure which can be brought to a diagonal form by a standard unitary transformation (i.e. a change of basis).

We wish to subject the fermion operators to a linear transformation

\[
\begin{pmatrix}
\hat{d}_1 \\
\hat{d}_2 \\
\hat{d}_1^\dagger \\
\hat{d}_2^\dagger
\end{pmatrix} = U
\begin{pmatrix}
\hat{c}_1 \\
\hat{c}_2 \\
\hat{c}_1^\dagger \\
\hat{c}_2^\dagger
\end{pmatrix}
\] (5)

and ensure that the new operators \(\{\hat{d}_1, \hat{d}_2^\dagger\}\) obey anti-commutation relations. It follows that the \(4 \times 4\) matrix \(U\) must be unitary. We write it in the block form

\[
U = \begin{pmatrix} U & V \\ V^\dagger & U^\dagger \end{pmatrix}
\] (6)

with each sub-matrix \(U, U', V, V'\) containing \(2 \times 2\) elements, so that \(\hat{d}_i = U_{ij} \hat{c}_j + V_{ij} \hat{c}_j^\dagger\) and \(\hat{d}_i^\dagger = V_{ij} \hat{c}_j + U_{ij} \hat{c}_j^\dagger\) (Einstein summation). It follows that \(U' = U^*\) and \(V' = V^*\) and the transformation matrix must have the following structure

\[
U = \begin{pmatrix} U & V \\ V^\dagger & U^\dagger \end{pmatrix}
\] (7)

Unitarity implies

\[
UU^\dagger + VV^\dagger = 1
\]

\[
UV^\dagger + VU^\dagger = 0,
\] (8)

with \(V^\dagger (U^\dagger)\) the transpose of \(V (U)\). We detail in appendices A and B how to choose \(U\) and \(V\) so that the transformed Hamiltonian is free from anomalous terms of the form \(d_1d_2\).

Then, the Hamiltonian can be rearranged to a normal-ordered form

\[
H = \Psi^\dagger \begin{pmatrix}
\epsilon_1' & 0 & 0 & 0 \\
0 & \epsilon_2' & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix} \Psi
\] (9)

where we introduce \(\Psi^\dagger = (d_1^\dagger, d_2^\dagger, d_1, d_2)\). We achieve the diagonalization by the transformation of the kind (5) with the structure of the unitary matrix

\[
\Psi'' = \begin{pmatrix} U'' & 0 \\ 0 & U'' \end{pmatrix}
\] (10)

This is, of course, a standard eigenvalue problem of a two-level system.

2.2.2. Chain. Our numerical diagonalization of the full Hamiltonian consists of iterative application of the procedure shown in the preceding section. Firstly, one singles out two orbitals in the Hilbert space, then applies the Bogoliubov transformation that removes pairing of the selected ‘dimer’, then transforms the remaining parts of the Hamiltonian accordingly.

Here we detail the outlined procedure. Let us consider a general Hamiltonian of Bogoliubov–de Gennes type

\[
H = \Gamma^\dagger \gamma \Gamma
\] (11)

where \(\Gamma^\dagger = (c_1^\dagger, \ldots, c_N^\dagger, c_1, \ldots, c_N)\) is a row vector of fermion operators labeled by indices of an orthonormal basis set (spin and orbital) and \(\gamma\) is a \(2N \times 2N\) matrix. The assignment of the matrix elements of \(\gamma\) is ambiguous and in what follows we will require the following \(N \times N\) block structure

\[
\gamma = \begin{pmatrix} h & b \\ -b & 0 \end{pmatrix}
\] (12)

with \(h^\dagger = h\) and \(b^\dagger = -b\). The fermionic operator algebra allows for linear automorphisms \(\Gamma = \gamma \Gamma\) by means of a unitary matrix \(\Upsilon\) with the \(N \times N\) block structure

\[
\Upsilon = \begin{pmatrix} U & V \\ V^\dagger & U^\dagger \end{pmatrix}
\] (13)

We wish to find a matrix \(\Upsilon\), which carries away all pairing and hopping terms from the Hamiltonian. In addition we demand that the transformed operators still obey fermionic anti-commutation relations, which again leads to the condition (8). It is important to note that this implies \(\Upsilon\) is unitary. However, an arbitrary unitary \(\Upsilon\) matrix will in general not adhere to the form (13) and therefore not conserve the fermionic anti-commutation relations. Therefore, just diagonalizing matrix \(\gamma\) will in general not lead to a valid solution. One may argue that any unitary matrix that diagonalizes \(\gamma\) should lead to the same solution. However, this does not apply here. The transformation we describe below will in general not lead to a completely diagonal matrix. Instead it will transform the matrix into a form where the off-diagonal symmetric part of \(h\) and the asymmetric part of \(b\) vanish. In addition the ‘0’ in (12) may not be zero. Therefore, the resulting matrix only leads to a Hamiltonian that is equivalent to a diagonal form for fermionic operators.

In order to ensure the structure (13) we developed an iterative procedure, sketched in the following steps (i)–(iii). Suppose that at the \(p\)th step we were given a matrix \(\mathcal{H}_p\)—of the form (12).

(i) We identify a pair of orbitals with the largest pairing, say \(m < n \leq N\). The operator set \(c_m, c_n, c_m^\dagger, c_n^\dagger\) is transformed to a new operator set \(c'_m, c'_n, c'_m^\dagger, c'_n^\dagger\), \(m < n \leq N\) in which the pairing vanishes. This amounts to solving the ‘dimer’ problem from section 2.2.1.

(ii) The matrix \(\mathcal{H}_p\) becomes \(\mathcal{H}_{p+1} = \mathcal{H}_p \mathcal{H}_p \mathcal{H}_p^\dagger\) when expressed in the new operator set, and the matrix \(\mathcal{H}_p\) does not mix operators with indices other than \(m\) or \(n\); in the dimer subspace the matrix \(\mathcal{H}_p\) has the same structure as in equations (8) and (7).
(iii) The Hermitian matrix $\cal H_{p+1}$ is to be brought to a form (12) by a permutation of fermionic operators. Note that this step eventually generates a $c$-number term to the Hamiltonian which can be discarded.

After all pairings are lower than a certain tolerance, we perform a basis change to rotate away hoppings. This can be achieved by the transformation matrix (13) with zero off-diagonal blocks and is a routine task. All results presented in this work were calculated by this iterative method; the Hamiltonian was thought converged if the absolute value of the highest pairing was smaller than $10^{-10} t$. We collect the product of all transformation matrices in order to calculate local quantities.

We emphasize that our diagonalization procedure can be applied to a wide class of systems, which are represented by Hamiltonians bilinear in fermionic operators, such as systems of arbitrary dimensionality, or disordered systems.

### 2.3. Spectral function

Let the Hamiltonian (1) be transformed to a diagonal form

$$H = \sum_i \hat{c}^\dagger_i \epsilon_i \hat{c}_i$$

by $d_i = \sum (U_i \hat{c}^\dagger_j + V_i \hat{c}^\dagger_j \hat{c}_j)$

The normal-component retarded Green’s function at site $i$ reads

$$G_2(\omega) = \left\langle \hat{c}_i^\dagger - \frac{1}{\omega - H + i\eta} \hat{c}_i + \frac{1}{\omega + H + i\eta} \hat{c}_i^\dagger \right\rangle.$$

The spectral function is given by the expression

$$A_2(\omega) = \frac{1}{\pi} \text{Im} \sum_i \left[ \frac{|U_i|^2}{\omega - E_i + i\eta} + \frac{|V_i|^2}{\omega + E_i + i\eta} \right]$$

where $\eta$ is a positive infinitesimal, which in the numerics will be substituted by a finite value of the order of the average level splitting around the Fermi level in the absence of superconductivity. Hereafter we shall use $\eta = 0.015 t$. The resulting spectra are deconvolved by the algorithm of [31] (poor man’s deconvolution).

### 3. Results

From now on, all numerical values of dimension energy (such as pairings, on-site energies, etc) will be in the units of $t$.

The Hamiltonian (1) is studied in two regimes:

(i) a resonant level coupled to a singlet-paired superconductor ($\Delta_T = 0, \Delta_S = 0.6$)

(ii) a resonant level coupled to a triplet-paired superconductor ($\Delta_S = 0, \Delta_T = 0.3$).

Thus, the superconducting bulk gap will be 2.4 in both cases. The rest of the chain Hamiltonian is parameterized as $\mu = 0$ and $t = 1$ as the unit of energy. In all cases, the superconducting chain has 200 sites. The RL is weakly coupled to the chain with $t_0 = 0.3$ and on-site energy $\epsilon_{0\sigma}$ will vary.

Hence, the case (ii) is in a topologically non-trivial phase [12] with Majorana modes. The first case is a topologically trivial superconducting state.

### 3.1. Behavior of local spectral function on gating

In figure 1 we show several spectral functions for case (i). There are no zero modes. The position of the highest peak coincides with the on-site energy of the resonant level $\epsilon_0$. Along with this RL peak, there is an Andreev reflected peak roughly at $\epsilon_0$. The mirroring behavior of the resonant and Andreev peak positions as the ‘gate’ varies is a known distinctive feature of the Andreev process. Finally, in the outside region $|E| > t$ two ridge-like features appear. These are the bulk features of an ordinary superconductor.

Now we proceed to case (ii), the topological superconductor, figure 2. A strikingly new feature is the zero-energy peak, which signals the spreading of the Majorana mode to the RL site. Note that the position of the RL is repelled from the bare value; the resonance center is shifted upwards. This can be understood as a delocalization of the Majorana mode: without the resonant state, the Hamiltonian in regime (ii) reduces to a spin-full Kitaev chain with zero modes localized at both edges. Coupling to the RL dilutes the Majorana state [28]; however, since its energy is fixed to zero, the coupling-induced splitting can affect the RL position only.

### 3.2. Magnetic field dependence of local spectral function

After seeing the distinct behavior of peaks under gating, we proceed to study the dependence of spectra in a weak magnetic field applied to the whole system. We introduce a homogeneous Zeeman field by substituting $\epsilon_{0\sigma} = \epsilon_0 + \sigma B/2$ and $\mu_\sigma = \mu + \sigma B/2$, $\sigma = \pm 1$ in the Hamiltonian (1). Hence, $B$ is the spin splitting of a single level.

In the singlet-paired case the RL and its Andreev reflected counterpart split, as shown in figure 3. Note that in the
Figure 2. Spectral function of a resonant level coupled to a triplet-paired superconductor chain with 200 sites. The resonant level couples via hopping $t_0 = 0.3$ to the chain. The three curves correspond to different on-site energies of the level.

Figure 3. Spectral function of a resonant level weakly coupled to a singlet-paired superconductor with 200 sites. The three curves represent different values of a homogeneous Zeeman field; each curve is a sum over two projections of spin. $B$ denotes the splitting of a single level and is expressed in multiples of the resonant level hopping $t_0$. For clarity, the spectra have been shifted vertically.

highest splitting $B = 2t_0$ an accidental zero-energy resonance forms from the overlap of two resonances. The magnitude of peak splitting obeys strictly the Zeeman term in the RL Hamiltonian. The observation of splitting is in agreement with recent quantum dot experiments [32].

As the last case, we consider the influence of the Zeeman field on the triplet-paired superconductor, case (ii). The pinning of the Majorana state to the zero energy (the chemical potential) is robust against a weak magnetic field, too. The magnetic field, however, splits the resonant and Andreev levels. Figure 4 shows the evolution of the spectral function for the Zeeman fields $B = 0, t_0$ and $2t_0$. The side peaks are clearly split while the central resonance stays almost intact. Again, all peaks ‘interact’ and apart from the previously mentioned shift of the Andreev and resonant levels off the zero energy, there is also a decrease in the spin splitting below the value given by $B$.

4 We remark that this part applies to the realizations of topological superconductivity where spin degeneracy remains.

4. Discussion

As stated in the introduction, zero-bias transport features can arise in solid state systems due to reasons unrelated to Majorana physics.

A thoroughly studied example is the Kondo effect. In the transport through quantum wires, Kondo physics could emerge due to enhancement of Coulomb interactions (due to reduced screening) or presence of a magnetic impurity in the wire. The spectral manifestation at low temperatures is the zero-energy Kondo resonance (width of the order of the Kondo temperature $k_B T_K$), and possibly charge peaks of the Anderson model. The side peaks need not be symmetric around the Fermi level and behave differently when external fields are introduced. A change of the gate voltage (on-site energy of the Anderson impurity) causes the lower and higher side peaks to move in the same direction, accompanied by a pronounced change in the width of the central (Kondo) resonance. This is in sharp contrast with the case of an RL coupled to a Majorana mode (compare to figure 2), where side peaks move off the zero bias symmetrically and the central resonance stays intact.

Further distinction emerges when studying the Zeeman splitting. Majorana resonance does not split even though the side peaks do (figure 4). The Kondo resonance, in contrast, is immune only for weak fields and splits when the Zeeman field becomes of the order of $k_B T_K$, i.e. of the order of the peak width. The resulting splitting of the zero-energy peak is then twice the Zeeman splitting. Hence, magnetic field and local gating are both independently sufficient to distinguish between both underlying mechanisms.

Finally, we remark that our calculations allow us to distinguish the Majorana mode from a Tamm–Shockley mode in a charge-density wave wire [24], because the latter is sensitive to a gate voltage.

5. Conclusions

We have developed an efficient numerical approach, able to treat hybrid inhomogeneous systems. Our method relies
on a fully fermionic formalism, that is, eigenstates of the Hamiltonian are fermions. We diagonalize the Hamiltonian by means of a unitary matrix and point out that the matrix structure must be restricted in order to satisfy anti-commutation algebra.

We have applied the method to the combined system of a resonant level (RL) and a superconducting chain. Regardless of the nature of pairing, gate voltage and magnetic fields couple to the RL, as we show in the analysis of the level’s spectral function. When triplet pairing is introduced, the local spectral function attains a zero-bias resonance, which does not react to external fields. In summary, the combined system allows us to prove that the perturbing field does couple to the system, at the same time demonstrating the presence of a Majorana mode.

Apart from direct access to spectral functions, the fermionic language could be conveniently used to calculate other local quantities, for instance wavefunctions of the zero modes. Alicea et al [4] have elaborated on the possibility of implementing quantum memory in a network of topological superconducting wires. Here, the braiding operation could be realized by changes in local gate voltages. Our method, straightforwardly extended to non-stationary regimes, offers a way to simulate braiding while tracking the Majorana state in real time.

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**Appendix A. Single angle Bogoliubov transformation**

In section 2.2.1 we introduced general conditions for the transformation matrix of the dimer fermion operators. In order to rotate the Hamiltonian in a particle conserving representation we have to rotate the asymmetric part of $B$ to zero. In the recipe described above we have reduced the problem to solving a two-site system which can be achieved via standard fermionic Bogoliubov transformation

\[
\begin{align*}
\hat{d}_1 &= \cos(\beta)\hat{c}_1 - \sin(\beta)\hat{c}_1^\dagger, \\
\hat{d}_2 &= \cos(\beta)\hat{c}_2 + \sin(\beta)\hat{c}_2^\dagger, \\
\end{align*}
\]

which fulfil the conditions (8). In matrix form they are given by

\[
U = \begin{pmatrix}
\cos(\beta) & 0 \\
0 & \cos(\beta)
\end{pmatrix}, \\
V = \begin{pmatrix}
0 & -\sin(\beta) \\
\sin(\beta) & 0
\end{pmatrix}.
\]

Using

\[
\tan(2\beta) = -\frac{2\Delta}{\epsilon + \epsilon'},
\]

the $\Delta$ contribution to Hamiltonian $H$ in (3) is transformed to zero.

**Appendix B. Two angle Bogoliubov transformation**

In addition to transforming the $\Delta$ part to zero, we can also rotate the $t$ contribution to zero by applying an additional rotation

\[
R = \begin{pmatrix}
\cos(\alpha) - \sin(\alpha) \\
\sin(\alpha) & \cos(\alpha)
\end{pmatrix},
\]

\[
U_R = R \cdot U, \\
V_R = R \cdot V,
\]

where the rotation angle is given by

\[
\tan(2\alpha) = -\frac{2t}{\epsilon - \epsilon'}.
\]

**Appendix C. Remarks on Nambu spinors**

In the case of s-wave pairing one usually resorts to Nambu spinors

\[
\Psi^\dagger_j = (\hat{c}_{j,\uparrow}^\dagger \hat{c}_{j,\downarrow}^\dagger - \hat{c}_{j,\downarrow} \hat{c}_{j,\uparrow}).
\]

Using the label $j = 2x$ for the up spins and $j = 2x + 1$ for the down spins this corresponds to a matrix representation using a transformation of the form

\[
\hat{U}_N = \begin{pmatrix}
1 & 0 \\
0 & U_N
\end{pmatrix},
\]

where $U_N$ is a block diagonal consisting of $2 \times 2$ rotation matrices with an angle of $\pi/2$. Using this transformation one is led to a matrix where the new $b$ block is actually symmetric. The disadvantage of the Nambu representation is that the conditions for preserving canonical anti-commutation relations are not as simple as equation (8) in our representation.

**Appendix D. Remarks on the numerics**

For the recipe of bringing the many site problem to diagonal form it is sufficient to use the single angle version. In our tests it turned out that the two angle version actually needs fewer iteration steps to converge. However, each step takes longer, because the number of vector operations is doubled. In return using the single angle version was typically faster.

One can also start the procedure by first rotating $b$ into a tridiagonal form using the algorithm of [27]. Moreover, an antisymmetric matrix can be transformed into a $2 \times 2$-block diagonal matrix $D = Q \cdot b \cdot Q^\dagger$ with $Q$ unitary [33, 34]. Since $D$ consists only of $2 \times 2$ and $1 \times 1$ blocks with a diagonal of zeros, $D^2$ is diagonal. Therefore we have

\[
D^2 = Q \cdot b \cdot Q^\dagger \cdot Q \cdot b \cdot Q^\dagger = Q \cdot b^2 \cdot Q^\dagger,
\]

where $Q$ is given by the diagonalization of $b^2$. Note that it is essential that $b$ is used in the antisymmetric form $b = -b^\dagger$. Starting our procedure with $U = Q$ and $V = 0$ leads to an initial $2 \times 2$-block diagonal matrix $b$ leading to an improved convergence rate in our tests.
References

[1] Majorana E 1937 Teoria simmetrica dell’elettrone e del positrone *Nuovo Cimento* 5 171–84
[2] Wilczek F 2009 Majorana returns *Nature Phys.* 5 614–8
[3] Beenakker C W J 2013 Search for Majorana fermions in superconductors *Annu. Rev. Condens. Matter Phys.* 4 113–36
[4] Alicea J, Oreg Y, Refael G, von Oppen F and Fisher M P A 2011 Non-abelian statistics and topological quantum information processing in 1D wire networks *Phys. Rev. Lett.* 106 220402
[5] Read N and Green D 2000 Paired states of fermions in solid state systems *Rep. Prog. Phys.* 75 076501
[6] Jiang L, Kitagawa T, Alicea J, Akhmerov A R, Pekker D, Refael G, Cirac J I, Demler E, Lukin M D and Zoller P 2011 Majorana fermions in equilibrium and in driven cold-atom quantum wires *Phys. Rev. Lett.* 106 220402
[7] Qi X L, Hughes T L and Zhang S C 2010 Chiral topological superconductor from the quantum Hall state *Phys. Rev. B* 82 184516
[9] Ivanov D A 2001 Non-abelian statistics of half-quantum vortices in p-wave superconductors *Phys. Rev. Lett.* 86 268–71
[10] Thomale R, Rachel S and Schmitteckert P 2013 Tunneling spectroscopy simulation of interacting Majorana wires *Phys. Rev. B* 88 161103
[11] Fu L and Kane C L 2008 Superconducting proximity effect and Majorana fermions at the surface of a topological insulator *Phys. Rev. Lett.* 100 096407
[12] Kitaev A Y 2001 Unpaired Majorana fermions in quantum wires *Phys.—USSR Phys. Z. Sowjetunion* 412–7
[13] Leijnse M and Flensberg K 2012 Introduction to topological insulators and Majorana fermions at the surface of a topological insulator *Semicond. Sci. Technol.* 27 124003
[14] Lutchyn R M, Sau J D and Das Sarma S 2010 Majorana fermions and a topological phase transition in semiconductor–superconductor heterostructures *Phys. Rev. Lett.* 105 077001
[15] Oreg Y, Refael G and von Oppen F 2010 Helical liquids and Majorana bound states in quantum wires *Phys. Rev. Lett.* 105 177002
[16] Mourik V, Zuo K, Frolov S M, Plissard S R, Bakkers E P A M and Kouwenhoven L P 2012 Signatures of Majorana fermions in hybrid superconductor–semiconductor nanowire devices *Science* 336 1003–7
[17] Das A, Ronen Y, Most Y, Oreg Y, Heiblum M and Shtrikman H 2012 Zero-bias peaks and splitting in an Al-InAs nanowire topological superconductor as a signature of Majorana fermions *Nature Phys.* 8 887–95
[18] Rokhinson L P, Liu X and Furdyna J K 2012 The fractional ac Josephson effect in a semiconductor–superconductor nanowire as a signature of Majorana particles *Nature Phys.* 8 795–9
[19] Deng M T, Yu C L, Huang G Y, Larsson M, Caroff P and Xu H Q 2012 Anomalous zero-bias conductance peak in a Nb–InSb nanowire–Nb hybrid device *Nano Lett.* 12 6414–9
[20] Cronenwett S M, Lynch H J, Goldhaber-Gordon D, Kouwenhoven L P, Marcus C M, Hirose K, Wingreen N S and Umansky V 2002 Low-temperature fate of the 0.7 structure in a point contact: a Kondo-like correlated state in an open system *Phys. Rev. Lett.* 88 226805
[21] Rokhinson L P, Guo L J, Chou S Y and Tsui D C 1999 Kondo-like zero-bias anomaly in electronic transport through an ultrasmall Si quantum dot *Phys. Rev. B* 60 R16319
[22] Tammi I 1932 Uber eine mogliche Art der Elektronenbindung an Kristalloberflachen *Phys. Z. Sowjetunion* 1 733–6
[23] Shockley W 1939 On the surface states associated with a periodic potential *Phys. Rev.* 56 317–23
[24] Gangadharaiah S, Trifunovic L and Loss D 2012 Localized end states in density modulated quantum wires and rings *Phys. Rev. Lett.* 108 136803
[25] Bagrets D and Altland A 2012 Class d spectral peak in majorana quantum wires *Phys. Rev. Lett.* 109 227005
[26] Bogolubov N N 1947 On the theory of superfluidity *J. Phys.—USSR Phys.—Usp.* 11 3
[27] Wimmer M 2012 Algorithm 923: efficient numerical computation of the pfaffian for dense and banded skew-symmetric matrices ACM Trans. Math. Softw. (TOMS) 38 30
[28] Gibertini M, Taddei F, Polini M and Fazio R 2012 Local density of states in metal-topological superconductor hybrid systems *Phys. Rev. B* 85 144525
[29] Sticlet D, Bena C and Simon P 2012 Spin and Majorana polarization in topological superconducting wires *Phys. Rev. Lett.* 108 096802
[30] Prada E, San-Jose P and Acedo R 2012 Transport spectroscopy of ns nanowire junctions with Majorana fermions *Phys. Rev. B* 86 180503
[31] Schmitteckert P 2010 Calculating Green functions from finite systems *J. Phys.: Condens. Matter* 22 012022
[32] Lee E J H, Jiang X, Houzet M, Aigoulo R, Lieber C M and De Franceschi S 2013 arXiv:1302.2611 [cond-mat.mes-hall]
[33] Ward R C, Liu X and Furdyna J K 1999 The fractional ac Josephson effect in a semiconductor–superconductor nanowire–Nb hybrid device *Nano Lett.* 12 6414–9
[34] Golub G H and Van Loan C F 1996 *Matrix Computations* 3rd edn (Baltimore, MD: Johns Hopkins University Press)