Majorana Zero Modes Modelling and Simulation

MT-507 - Modelling and Simulation in Material Science (JAN-JUNE 2025)

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Submitted to: Dr. Dube Dheeraj Prakashchand Sir

Submission Date: 10-5-25

Abstract

This presentation explores the modeling and simulation of Majorana Zero Modes (MZMs) in the 1D Kitaev chain, a topological superconductor. We cover:

- Theoretical framework of the Kitaev chain model
- Data generation workflow using the Kwant package
- Analysis techniques, including machine learning predictions
- Diagnostic visualizations to identify MZM signatures
- Use of gate voltage as a tunable parameter to distinguish the presence of trivial and topological phases

Our approach can be used for applications in topological quantum computing (e.g., Microsoft Majorana 1), offering insights into quantum materials design.

Literature Review on MZM Detection

- **Introduction**: Overview of existing research on Majorana zero modes (MZMs) in superconductor-semiconductor systems.
- **Key References**:
  - Mourik et al. (2012) – Experimental ZBPs via gate and magnetic field.
  - Cheng et al. (2023) – ML-based ZBP classification using conductance maps.
  - Others – Alternative setups or detection schemes.
- **Relevance to Our Work**: These studies support our field-free, ML-assisted MZM detection strategy.

(Updated references integrated in next slide)

Comparison of Two MZM Detection Papers

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Aspect	Mourik et al. (2012)	Cheng et al. (2023)
Objective	Detect MZMs experimentally via zero-bias peaks (ZBPs) in InSb nanowires	Classify MZM presence using M on simulated and real ZBP co ductance data
Approach	Tunnel spectroscopy with gate-controlled chemical potential and external magnetic field	Tight-binding simulations + X Boost classifiers on noisy condu tance maps
Key Parameters	- Strong Rashba spin-orbit coupling - Zeeman field B for topological phase - Gate voltages to tune μ and tunnel barrier	- Simulate BdG Hamiltonians - Include disorder + Gaussian noise - Sweep V_{bias} and μ

Our Approach to Detect MZMs

- **Objective**: Detect Majorana zero modes (MZMs) in a superconductor-semiconductor nanowire system (e.g., InSb/Al).
- **Method**: Simulate the nanowire system, generate conductance maps, and use ML to classify maps as topological or trivial.
- **Key Signature**: A zero-bias peak (ZBP) at $V_{\text{bias}} = 0$ indicates MZMs.
- **Simulation Parameters**:
  - t: Hopping parameter — electron tunneling between lattice sites
  - μ: Chemical potential — tuned via gate voltage
  - Δ: Superconducting gap — controls pairing energy
  - `disorder_strength`: Simulated on-site noise to mimic disorder
  - `local_potential`: External electrostatic confinement
  - V_{bias}: Source-drain bias — controls tunneling energy
- **Conductance**: $\frac{dI}{dV} = G_0 \cdot T(E), \quad G_0 = \frac{2e^2}{h}$

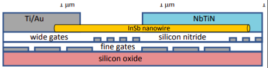
Data Generation and Experimental Setup

- **Data Generation**:
  - Simulate nanowire with leads, generating 4000 conductance maps on 30×30 grid (μ vs. V_{bias})
  - Add disorder to simulate experimental noise
- **Experimental Setup**:
  - 1D InSb wire with Al superconductor; length $= 1\ \mu$m
  - Au leads; gate voltage controls μ from -60 meV to 60 meV
  - Device measures I, computes $\frac{dI}{dV}$

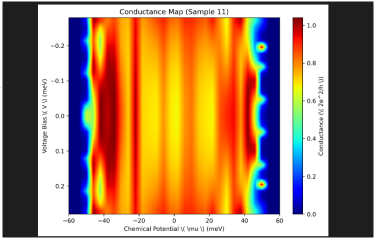
Mechanism of the Fermi Level

- **Fermi Levels at $V_{\textbf{bias}} = 0$**:
  - Leads: $E_F = 0$ (reference energy)
  - Nanowire: $E_F = \mu$, tuned by gate voltage V_g
- **Tunneling Condition for MZMs**:
  - MZMs exist at $E = 0$ in topological phase
  - $\mu \approx 0$ aligns nanowire with leads $\rightarrow$ **ZBP appears**
  - $\mu = \pm 60$ meV misaligns levels $\rightarrow$ **ZBP disappears**
- **Effect of $V_{\textbf{bias}}$**:
  - ± 0.28 meV shifts leads' Fermi levels away from $E = 0$
  - Tunneling misses MZMs $\rightarrow$ **No ZBP**
- **Gate Voltage Control**:
  - $\mu = e \cdot V_g \cdot C$; positive V_g increases μ
  - Controls electron density and energy level alignment

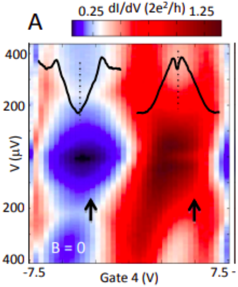
Visuals: Setup and Conductance Maps



Experimental Setup



Our Conductance Map



Paper Conductance Map

- **ZBP at center** → MZM present
- **No ZBP** or split peak → Trivial phase

Data-Generation Workflow

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Step	Description	Output
1. Parameter Selection	Choose chain length L, hopping t, chemical potential μ, pairing Δ	(L, t, μ, Δ)
2. Construct BdG Matrix	Build the $2L \times 2L$ BdG Hamiltonian in Nambu basis	$\mathcal{H}_{\text{BdG}}$
3. Diagonalization	Numerically diagonalize $\mathcal{H}_{\text{BdG}}$ via eigh	Eigenvalues $\{E_n\}$, Eigenvectors $\{\Phi_n\}$
4. Zero-Mode Identification	Select mode(s) with $\lvert E_n \rvert \approx 0$ (Majorana candidates)	Φ_{zero}
5. Localization Length	Compute $\lvert\psi_j\rvert^2 = \lvert u_j\rvert^2 + \lvert v_j\rvert^2$ and fit $\exp(-2j/\xi)$	ξ
6. Data Storage	Aggregate all parameters, spectra, wavefunctions, ξ	HDF5 record per sample

1D Kitaev Chain Hamiltonian

The 1D Kitaev chain is a model for topological superconductors, describing a spinless chain of N lattice sites with nearest-neighbor hopping and p-wave pairing. The Hamiltonian captures the physics of Majorana Zero Modes (MZMs), which are zero-energy edge states with potential applications in topological quantum computing.

$$H = -\mu \sum_{j=1}^{N} c_j^\dagger c_j - t \sum_{j=1}^{N-1} \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) + \Delta \sum_{j=1}^{N-1} \left(c_j c_{j+1} + c_{j+1}^\dagger c_j^\dagger \right).$$

Parameter Sweep for Dataset Generation

To study MZM behavior, we sweep system parameters over uniform grids using `linspace`:

$$\mu \in [\mu_{\text{min}}, \mu_{\text{max}}], \quad t \in [t_{\text{min}}, t_{\text{max}}], \quad \Delta \in [\Delta_{\text{min}}, \Delta_{\text{max}}],$$

$$B \in [B_{\text{min}}, B_{\text{max}}], \quad \alpha \in [\alpha_{\text{min}}, \alpha_{\text{max}}].$$

The dataset includes:

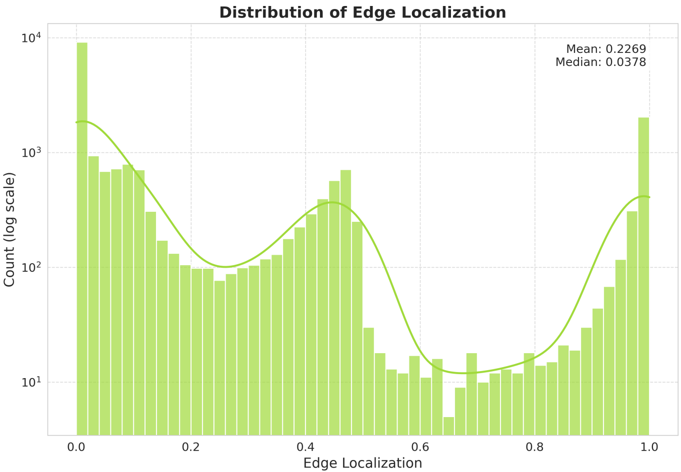
$$\big(\mu, t, \Delta, B, \alpha; E_n, \psi_n, \xi, \nu\big),$$

enabling analysis of MZM occurrence across parameter space.

Variable Definitions

- $c_j^\dagger, c_j$ Creation/annihilation operators at site j.
- μ Chemical potential, controlling particle density.
- t Hopping amplitude between nearest neighbors.
- Δ p-wave pairing amplitude, enabling superconductivity.
- N Number of lattice sites in the chain.
- E_n, ψ_n Eigenvalues/eigenvectors of H_{BdG}, describing quasiparticles.
- ξ Localization length, measuring edge mode confinement.
- ν Winding number, indicating topological phase.
- B Zeeman field strength, introducing magnetic effects.
- α Spin-orbit coupling strength, affecting electron spin.

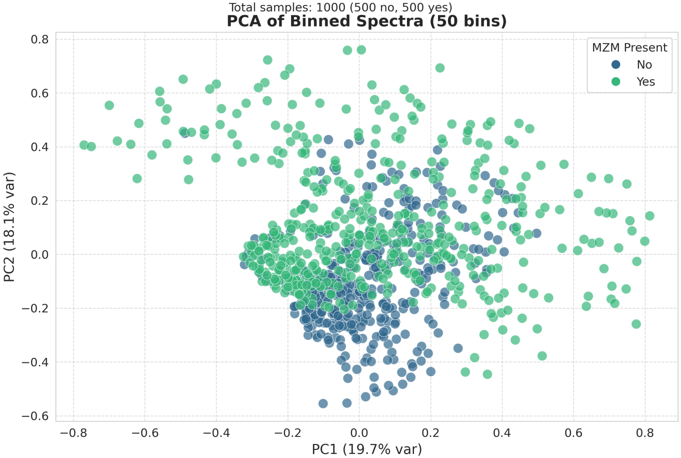
Edge-Localization Histogram



Edge-localization histogram. The x-axis is the normalized localization metric ($0 =$ bulk; $1 =$ edge), and the y-axis shows the sample count (log scale).

This histogram reveals an almost trimodal-like distribution, indicating states are either bulk-like or edge-localized, with MZMs appearing at the edge (metric ≈ 1).

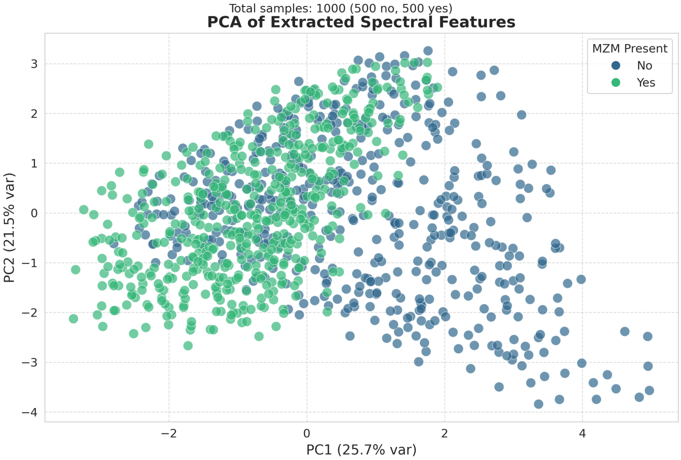
PCA of Raw Binned Spectra



PCA of raw binned spectra (50 bins). PC1 and PC2 capture 19.7% and 18.1% of variance.

Using raw spectra results in poorer class separation compared to engineered features, highlighting the importance of feature engineering for MZM detection.

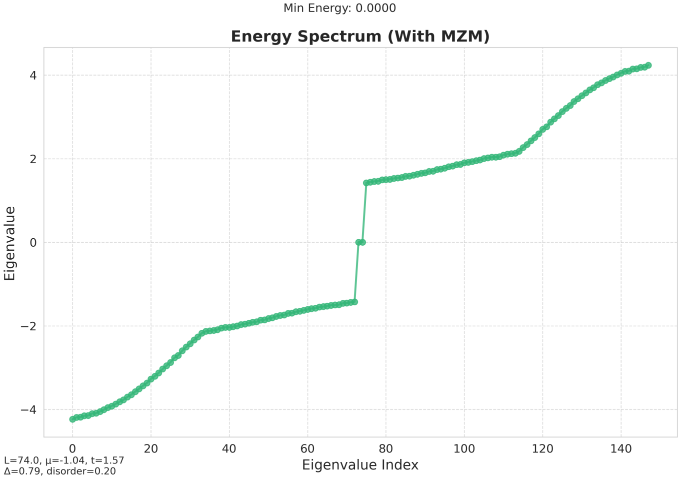
PCA of Engineered Spectral Features



PCA of engineered spectral features. Axes are the first two principal components (PC1, PC2), capturing 25.7% and 21.5% of variance.

The clear separation in this PCA plot shows that engineered features effectively distinguish MZM-hosting parameter sets, with PC1 and PC2 as arbitrary projections.

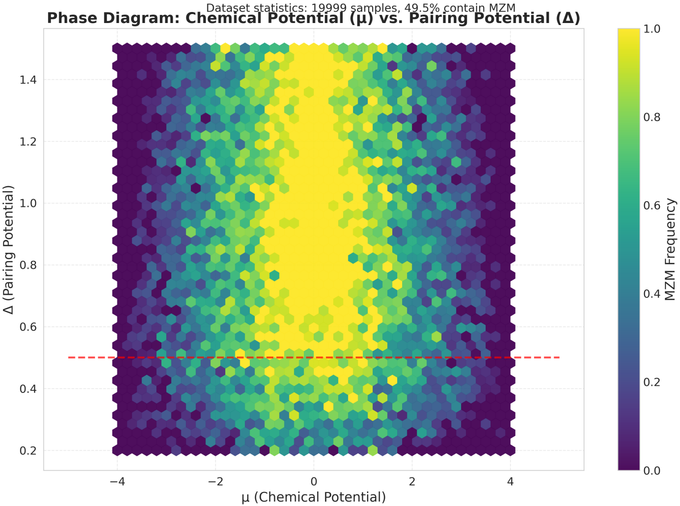
Energy Spectrum with MZM



Energy spectrum with an MZM. The x-axis indexes sorted eigenvalues; the y-axis gives eigenvalues in energy units (e.g., meV).

The spectrum shows a pair of states at or near zero energy, a hallmark of MZMs, distinguishing them from bulk states with finite energy gaps.

Phase Diagram in (μ, Δ) Plane



Phase diagram in the (μ, Δ) plane. The x-axis is μ (eV), the y-axis is Δ (eV), and color encodes MZM occurrence frequency.

This hexbin plot maps MZM occurrence, with the red dashed line at $\Delta = 0.5$ highlighting a region of high MZM probability, guiding parameter selection.

Summary of MZM Diagnostics

The diagnostics confirm MZM presence through:

- Bimodal edge-localization (histogram).
- Clear separation in PCA with engineered features vs. raw spectra.
- Zero-energy modes in the spectrum.
- High MZM occurrence in specific (μ, Δ) regions.

These results validate the Kitaev chain as a platform for studying topological superconductivity.

booktabs caption listings

Input: A 5-dimensional feature vector $\mathbf{x} = [L, \mu, t, \Delta, \sigma_{\text{dis}}]$.

Output: An 181-dimensional vector $[\ell,\ \lambda_1, \lambda_2,\ \ldots, \lambda_{180}]$, where ℓ is the scalar edge-localization score and $\{\lambda_i\}$ are the BdG eigenvalues. We mask the output vector while training as the output is dependent on L. **Dataset Generated:** 2,00,000 training and 30,000 training Dataset generated and stored in HDF5 file.

Table: Architectural breakdown of `EnhancedBdGPredictor`.

Stage	**Layer Type**	**In→Out**	**Remarks**
Input	Linear	5→256	Linear + GELU + Dropout
FeatureExtractor	Linear	256→512	Residual projection, LayerNorm, Dropout
Edge-Loc Head	Linear	512→128	GELU, LayerNorm
	Linear	128→1	Scalar output
Spectrum Head	Linear	512→512	GELU, LayerNorm
(conv variant)	Conv1D	16 ch $\times$32 len	Residual conv block
	Linear	512→180	Eigenvalue outputs

Simulation of 1D Majorana Zero Modes in the Kitaev Chain

To generate 1D Majorana Zero Mode (MZM) data for the Kitaev chain, we employed the Kwant software package [2], a powerful tool for quantum transport simulations. The Kitaev chain model, originally proposed by Alexei Kitaev [1], describes a 1D p-wave superconductor that hosts MZMs at its ends under certain conditions. Our methodology for simulating this model and observing MZMs was informed by several key studies. For instance, [3] utilizes Kwant to simulate topological systems and detect MZMs via machine learning techniques applied to zero-bias peak measurements. Additionally, [4] provides the theoretical foundation for realizing MZMs in 1D systems, which aligns with the Kitaev chain model implemented in our simulations. The Kwant documentation and tutorials [5] further supported the practical implementation of these simulations.

References

- A. Yu. Kitaev, "Unpaired Majorana fermions in quantum wires," Physics-Uspekhi, vol. 44, no. 10S, pp. 131–136, 2001. DOI: 10.1070/1063-7869/44/10S/S29
- C. W. Groth, M. Wimmer, A. R. Akhmerov, and X. Waintal, "Kwant: a software package for quantum transport," New Journal of Physics, vol. 16, no. 6, p. 063065, 2014. DOI: 10.1088/1367-2630/16/6/063065
- M. Cheng, R. Okabe, A. Chotrattanapituk, and M. Li, "Machine learning detection of Majorana zero modes from zero-bias peak measurements," Matter, vol. 7, no. 7, 2024. DOI: 10.1016/j.matt.2024.05.028
- R. M. Lutchyn, J. D. Sau, and S. Das Sarma, "Majorana fermions and a topological phase transition in semiconductor-superconductor heterostructures," Physical Review Letters, vol. 105, no. 7, p. 077001, 2010. DOI: 10.1103/PhysRevLett.105.077001
- Kwant development team, "Kwant: a software package for quantum transport," `https://kwant-project.org/`, accessed 2023.