Topological Invariants and Unconventional Superconducting Pairing from Density of States via Machine Learning

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Abstract

The competition between magnetism and superconductivity can result in unconventional and topological superconductivity, where the presence of Majorana edge states and odd-frequency pairing poses a significant experimental challenge. In this work, we study a two-dimensional lattice model of a superconductor with spin-orbit coupling and randomly distributed magnetic impurities. We compute the Bott index, a real-space topological invariant, and map the phase diagram indicating both topologically trivial and nontrivial phases. We employ machine learning (ML) algorithms to predict the Bott index from the local density of states (LDOS) at zero energy, achieving high accuracy. Additionally, we train ML models to estimate the magnitude of odd-frequency pairing in the anomalous Green's function. Our results suggest that once trained, these ML models can predict the number of Majorana edge states and the strength of odd-frequency pairing in real materials using LDOS data obtained from scanning tunneling spectroscopy.

Key Results

The Hamiltonian for the system is given by:

$$H = \sum_r \left[\psi_r^\dagger(-t\tau_z + i\alpha\sigma_y\tau_z)\psi_{r+\hat{e}_x} + \psi_r^\dagger(-t\tau_z - i\alpha\sigma_x\tau_z)\psi_{r+\hat{e}_y} + h.c.\right] + \sum_r \psi_r^\dagger(-\mu\tau_z + \Delta\tau_x - J_r\sigma_z)\psi_r, \quad (1)$$

where ψ_r is the Nambu spinor, τ_a and σ_a are Pauli matrices, and the parameters t, μ, Δ, α, and J correspond to hopping, chemical potential, mean-field superconducting pairing, Rashba spin-orbit coupling, and exchange coupling, respectively. The Bott index, which we use to identify topological phases, is defined as:

$$B = \frac{1}{2\pi}\text{Im}\{\text{Tr}[\log(UVU^\dagger V^\dagger)]\}, \quad (2)$$

where U and V are unitaries derived from the operators X and Y projected onto the occupied states.

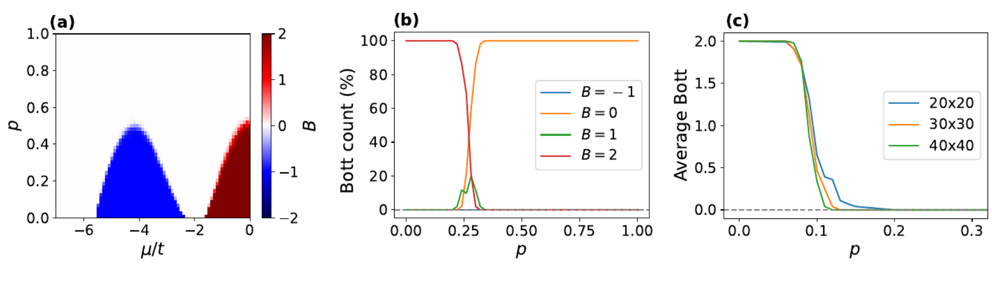

Figure 1: Phase diagram showing the topological phases as a function of the chemical potential μ and disorder parameter p, characterized by the Bott index B. For more details, check arXiv: 2408.16499.