Surface Results of a Superconductor based on a Higher-Order Topological Insulator $MoTe_2$

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I. INTRODUCTION

Higher-order topological insulators (HOTIs) are topological insulators (TIs) with a dimensional difference between the bulk and zero energy state by more than one. This will lead to an interesting system such as a 3-dimensional system with conducting corner or hinge states, or a 2-dimensional system with conducting corner states. Majorana fermions are particles which are their own anti-particle, it is expected to arise in the surface of topological superconductors.

This report is ordered as follows. Using the bulk Hamiltonian of the 3-dimensional metal dichalcogenides $MoTe_2$ given in Ref.[1], the system is expanded using the Bogliubov-de Gennes (BdG) Hamiltonian. The surface Hamiltonian is found by linearizing the Hamiltonian near the gap closing point via the methods similar to that of Ref.[2]. Wavefunctions of the zero-energy states are seen to determine whethere they are Majorana fermions. Finally, corner states given by the surface Hamiltonian will be compared to that of the tight-binding (TB) calculations. These calculations will be performed for s-wave pairing systems.

II. SURFACE HAMILTONIAN

The bulk Hamiltonian of a $MoTe_2$ system is given via [1]

$$H_{\text{SOTI}} = H_0 + H_{\text{SOC}} + V, \tag{1}$$

with each term being

$$\begin{aligned} H_0 &= \left[m + \sum_{i=x,y,z} t_i \cos k_i \right] \tau_z + \lambda_x \sin k_x \tau_x + \lambda_y \sin k_y \tau_y \mu_y \\ H_{\text{SOC}} &= \lambda_z \sin k_z \tau_y \mu_z \sigma_z \\ V &= m_l \tau_z \mu_z + m_s \mu_x. \end{aligned}$$

τ, μ are Pauli matrices indicating orbital degrees of freedom and σ indicate the spins. The system inclues the inversion symmetry $P = \tau_z$ and time-reversal (TR) symmetry $T = i\tau_z\sigma_y K$.

The BdG Hamiltonian is expanded on using H_{SOTI} as

$$H_{\text{BdG}} = \begin{pmatrix} H_{\text{SOTI}} - \mu & \Delta(\mathbf{k}) \\ \Delta(\mathbf{k})^\dagger & -H_{\text{SOTI}}^T + \mu \end{pmatrix} \tag{2}$$

with $\Delta(\mathbf{k})$ being the pairing functions. The chemical potential of the system μ is such that it is smaller than the conduction band bottom of H_{SOTI}.

The basic principle of finding the surface Hamiltonianis similar to finding the domain wall bound states of a 1-dimensional Su-Schrieffer-Hegger model. That is, expressing the Hamiltonian in the space of the occupied states. The crystal momenta is written in the cylindrical coordinates as $\mathbf{k} = (k_\perp \cos\phi - k_\parallel \sin\phi, k_\perp \sin\phi + k_\parallel \cos\phi, k_z)$. This keeps the system periodic in the z-direction while having one good quantum number along the edge of the surface and renders only $k_\perp$ into an operator $-i\partial_{r_\perp}$. Using a trial wavefunction $|\psi(r_\perp)\rangle = \exp\left[-\frac{1}{2}Mr_\perp^2\right]|u\rangle$, the surface Hamiltonian of H_{BdG} will be given as

$$H_{\text{S}} = -k_\parallel \xi_z \sigma_y - (m_s \cos\phi - m_l \sin\phi)\,\xi_z\,(\cos\phi\sigma_x + \sin\phi\sigma_z) + \lambda_z k_z \tau_z\,(\sin\phi\sigma_x - \cos\phi\sigma_z) + \mu\xi_z + \Delta, \tag{3}$$

with ξ_i, τ_i, σ_i indicating the Nambu space, spin and orbital, respectively. The results of the pairing terms are given via Δ.

III. RESULTS OF THE PAIRING FUNCTIONS

The pairing potential is given by the pairity operator, and the given pairing is either odd- or even-pairity determing on the eigenvalue of the pairing potential. In short, $\tau_z\Delta(\mathbf{k})\tau_{\mathbf{z}} = \boldsymbol{\Delta}(\mathbf{k})$ will be even parity and $\tau_z\Delta(\mathbf{k})\tau_{\mathbf{z}} = -\boldsymbol{\Delta}(\mathbf{k})$ will be odd-parity. Fermion statistics, $\Delta(\mathbf{k})^{\mathbf{T}} = -\boldsymbol{\Delta}(-\mathbf{k})$ is also satisfied. The resulting pairing functions and the resulting Δ regarding the surface Hamiltonian, and the dispersion of the hinges resulting from the surface Hamiltonians are given in Table 1.

	Pairing	Δ	Band
$\tau_z\mu_y\sigma_z$	1	$\Delta_0\xi_x\tau_z\sigma_y$	$\pm\mu\pm\lambda_z k_z$
$\tau_z\mu_y\sigma_x$	1	$-\Delta_0\xi_x\tau_x\sigma_y$	$\pm\mu\pm\lambda_z k_z$
$\tau_x\mu_x\sigma_y$	-1	$\Delta_0\xi_y\tau_y(\cos\phi\sigma_x+\sin\phi\sigma_z)$	$\pm\mu\pm\lambda_z k_z$
τ_y	-1	$\Delta_0\cos\phi\xi_y\sigma_y$	$\pm\mu\pm\lambda_z k_z$
$\tau_x\sigma_y$	-1	$\Delta_0\cos\phi\xi_y\tau_y$	$\pm\sqrt{\Delta_0^2\cos^2\phi+(\lambda_z k_z\pm\mu)^2}$
$\tau_x\mu_z\sigma_y$	-1	$\Delta_0\xi_y\tau_y(\sin\phi\sigma_x-\cos\phi\sigma_z)$	$\pm\sqrt{\Delta_0^2\cos^2\phi+(\lambda_z k_z\pm\mu)^2}$

TABLE I. **Pairing Results** The results of possible s-wave pairing. The pairing column indicates even- (1) and odd- (-1) pairing functions. Δ_0 is a constant given for the s-wave pairing function and Δ is the Δ term given in H_S. Band indicates the dispersion of the hinge states given by the surface Hamiltonian.

The Band results of Table 1 gives insight to the wavefunction of the hinge states. $\pm\mu\pm\lambda_z k_z$ gives a hinges where the pairing is non-existent. Threfore the hinges are at zero-energy, however are not Majorana fermions. These will be denoted as metallilc, as electrons, not Majorana fermions are charge carriers. The other case has Δ_0 in its value, which indicates that there is pairing. Indeed, it is only with $\tau_x\sigma_y, \tau_x\mu_z\sigma_y$ that there is a mix of the states in Nambu space. The problem aries however in the form of the hinge dispersion. It can not be zero as the hinges require $\cos\phi=\frac{1}{\sqrt{2}}$. These states will be denoted as gapped states. Fig.1 compares the analytical results of H_{BdG} and Band result of Table 1 with that of the TB method. It shows that the analytical results match well with those of the numerical TB results.

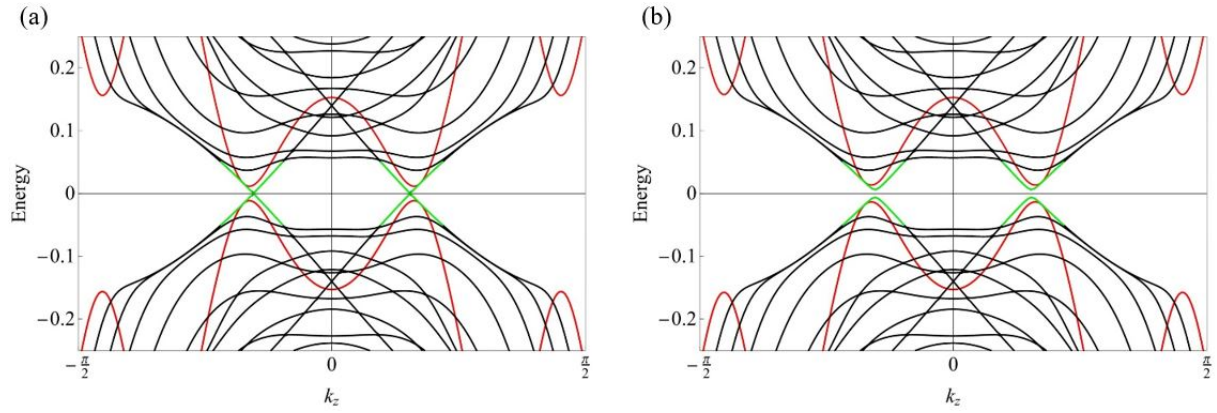


FIG. 1. **Band Results** Dispersion results given by H_{BdG}, dispersion of the hinge states and TB method given in red, green and black, respectively. (a) is the band results of metallic cases, while (b) gives the results for gapped cases. The parameters are $t_x=t_y=1, t_z=2, \lambda_x=\lambda_y=1, \lambda_z=0.3, m=-3, m_l=m_s=0.5, \Delta_0=0.02, \mu=0.14$

IV. CONCLUSION

In closing this report gave the surface Hamiltonian and the resulting zero energy states of the superconducting state of $MoTe_2$. The existing hinge-states of the s-wave pairing states are all metalic. Majorana states can be found in the hinges, however they are not zero-energy states and only exist in the odd-pairity case. It is therefore necessary to change the pairings into anisotropic pairings such as p-wave pairing and explore the results to check whether there are zero-energy hinge Majorana states.

[1] M. Ezawa, Sci. Rep. **9**, 5286 (2019)
[2] F. Schindler, J. Appl. Phys. **128**, 221102 (2020)