

Effect of Inversion Asymmetry on Quantum Confinement of Dirac Semimetal Cd_3As_2

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The discovery of the 3D Topological Dirac semimetal Cd_3As_2 presents a new class of semimetals because of its unique electronic structure and transport properties, demonstrating potential in novel topological devices. Promising properties of Cd_3As_2 include its topological surface states, ultrahigh electron mobility, and linear band dispersion. We evaluated the effect of inversion asymmetry on quantum confinement of Cd_3As_2 by measuring its electronic properties with and without hybridization through the quantum transport simulation package Kwant. Due to confinement, Cd_3As_2 exhibits a similar state to a 3D topological insulator because the transport in the bulk state becomes gapped, causing the surface state to dominate transport similar to 3D topological insulators. Thus, we can compare transport properties and band structure of Cd_3As_2 with other known 3D topological insulators such as HgTe and $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ through the analysis of previous electrostatic gating studies. We observe the lifting of the spin degeneracy due to inversion asymmetry and demonstrate that Cd_3As_2 provides a promising platform for topological device applications.

Keywords: Landau levels, Dirac hamiltonian, intersurface hybridization, inversion symmetry, topological insulator

I. INTRODUCTION

In recent years, three-dimensional (3D) topological Dirac semimetals have been an incredibly active topic in the field of condensed matter physics, largely due to its non-trivial electronic structure and special transport properties. These characteristics include high mobility and conductivity as well as a linear band dispersion, leading to gapless conduction in the surface states [1]. Furthermore, Dirac semimetals exhibit backscattering suppression due to their protection of time reversal symmetry, creating topological surface states with dissipationless transport of electrons [1]. Cd_3As_2 , a stable 3D topological Dirac semimetal, has attracted attention in developing logical devices since its surface states provide robust, gapless transport even under quantum confinement. The electronic transport on the surface states could also be turned on and off electrically, which is desirable in various spintronics applications [2,5].

Under quantum confinement, the Dirac semimetal Cd_3As_2 exhibits similar properties to a 3D topological insulator [2]. The bulk state of Cd_3As_2 exhibits minimal influence on the overall electronic transport throughout the material [4]. In other words, the surface states dominate most of the electronic transport, allowing the thickness of the thin film to be a tunable property of the semimetal [5]. Under quantum confinement, the surface states are extremely close to each other and could potentially impact each other through a phenomenon known as hybridization. Furthermore, because the substrate that the thin film of Cd_3As_2 is grown on could be different from its cap, there is a difference in chemical potential between the top and

bottom surfaces, known as structural inversion asymmetry. Previous experiments have confirmed the Dirac semimetal character of Cd_3As_2 , but current theories lack understanding of electronic interaction under inversion symmetry and hybridization of surface states.

In this study, we analyze the effect of structural inversion symmetry breaking on the quantum system by varying the chemical potential on the surface states and recording changes in the Landau level index diagram and energy-momentum dispersion of the semimetal. We study the effect of symmetry breaking under both hybridization and without hybridization to see how electrons interact under the two different circumstances. Using the Python package Kwant, we first simulate electronic transport under inversion symmetry breaking and then compare results with experimental data on 3D topological insulators such as HgTe and $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ [6]. By observing how these electrons interact under these conditions, we demonstrate that the Dirac semimetal Cd_3As_2 can be manipulated by changing the potential difference of the top and bottom surfaces. This difference in potential can be induced by an external electric field which lifts the spin degeneracy, creating spin-polarized states. We could then obtain full electric control of electronic transport of the system which provides a promising platform for developing topological field effect transistors and spintronics applications.

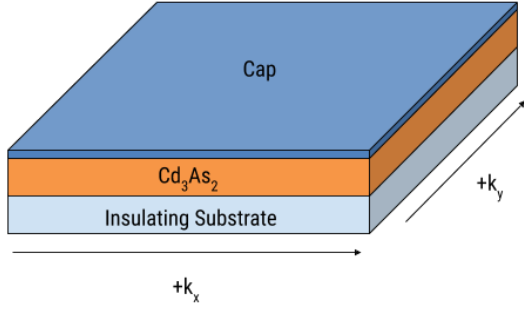


FIG. 1. Thin film of Dirac semimetal Cd_3As_2 . Different top and bottom surface materials creates a potential difference which breaks inversion symmetry ($\Delta_i \neq 0$). This demonstrates that we could change the inversion symmetry term by changing the material of the top and bottom surfaces or increase hybridization ($\Delta_h \neq 0$) by decreasing the thickness of the thin film.

II. THIN FILM AND METHODOLOGY

To analyze the confinement effects on the surface states of a thin film of Cd_3As_2 , we utilize a two Dirac-cone model representing the top and bottom surface states. Due to quantum confinement, we can neglect the contribution of the bulk state on the overall electronic transport of the system [8]. Thus, we can write our effective Hamiltonian in terms of a four state basis: $|\alpha, \sigma\rangle$ where $\alpha = \pm$ represents the top and bottom surface states and $\sigma = \uparrow, \downarrow$ denotes the spin [7]. Using this four state basis, We can write our Dirac Hamiltonian equation as

$$\begin{aligned} \mathcal{H} = & \hbar v_f \begin{pmatrix} (k_x \sigma_y - k_y \sigma_x) & 0 \\ 0 & -(k_x \sigma_y - k_y \sigma_x) \end{pmatrix} \\ & + \begin{pmatrix} \Delta_i & 0 \\ 0 & -\Delta_i \end{pmatrix} \\ & + \begin{pmatrix} 0 & \Delta_h \\ \Delta_h & 0 \end{pmatrix} \\ & + \begin{pmatrix} g^* \mu_B B_0 \sigma_z & 0 \\ 0 & g^* \mu_B B_0 \sigma_z \end{pmatrix} \end{aligned} \quad (1)$$

where \hbar is the reduced Planck's constant, v_f is the Fermi-velocity, k_x, k_y is the momentum in the x,y direction, Δ_i is the inversion symmetry breaking term, Δ_h is the hybridization term, g^* is the g-factor of Cd_3As_2 , μ_B is the Bohr magneton, and B_0 is the external magnetic field. To break the inversion symmetry of the two-state system, the top and bottom surface must have different chemical potentials which can be induced by having different materials on the top and bottom surfaces which increases Δ_i [7]. We could also manipulate Δ_h by varying

the thickness of the thin film causing different amounts of interaction between the top and bottom surface [7].

In order to study the effect of the manipulation of Δ_i and Δ_h , we utilize a quantum transport simulation to model these effects. We first test the effect of changes to inversion asymmetry without hybridization then test the effect of inversion asymmetry under hybridization for various values. We create our quantum system by first discretizing the continuous Hamiltonian to follow a tight-binding model. Next, we utilize Kwant to solve for the Landau levels as a function of a varying magnetic field. To plot the energy-momentum dispersion, we create a template of the Hamiltonian and attach a lead to the system which will allow us to plot the band structure of the system against the momentum. Analyzing changes in the energy-momentum dispersion and Landau levels due to different values of Δ_i and Δ_h will allow us to characterize electronic transport and band structure under these conditions.

After testing and understanding changes in the band gap and electronic transport of the Dirac semimetal due to inversion asymmetry breaking and hybridization, we then compare our simulation results to previous experimental data [4,16-18]. We analyze the Landau level index diagram and energy-momentum dispersion for different 3D topological insulators such as HgTe and $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$. After verifying our simulation results and understanding electronic interactions under inversion asymmetry breaking and hybridization, we then propose possible novel topological devices that manipulate these terms.

III. RESULTS AND DISCUSSION

1. Model for the Dirac Semimetal Cd_3As_2

After simulating electronic transport in a quantum system following the effective Hamiltonian in (1), we plot the system in two cases: 1. system with broken inversion symmetry without hybridization and 2. system with broken inversion symmetry and hybridization.

We take for the first case that the thin film has a thickness of 60-70nm so that it is under quantum confinement but the hybridization term $\Delta_h \approx 0$ since the two surface states will not significantly interact with each other [9]. We assume for the second case that the thin film has a thickness $\leq 15\text{nm}$, signifying that the system is under quantum confinement and that the hybridization term Δ_h significantly affects the system. We also take the g-factor of Cd_3As_2 to be 4.5 and the Fermi-velocity $v_f = 8.8 * 10^5$ [4]. In both cases, we take the magnetic field B to be in the (001) direction for values 0-2T, making the Zeeman-type term significant to the energy levels [9].

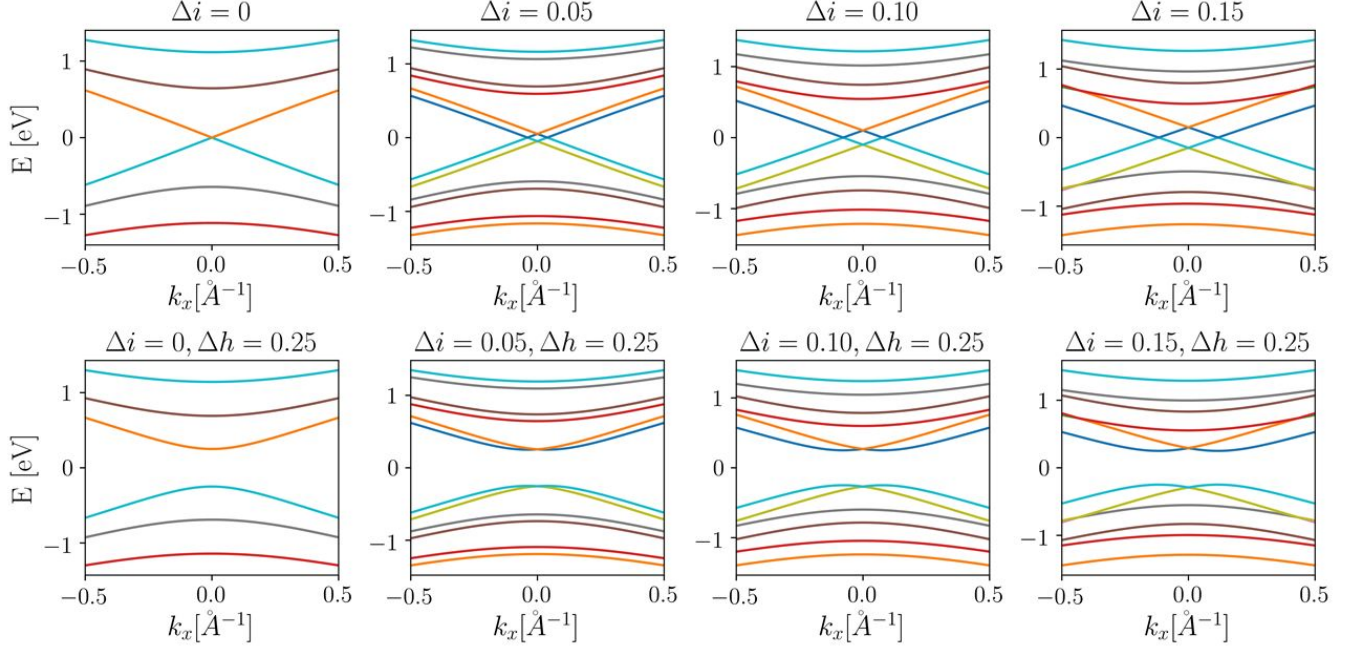


FIG. 2. First row: Energy-Momentum Dispersion with inversion asymmetry but no hybridization Second row: Energy-Momentum Dispersion with inversion asymmetry and hybridization

2. Energy-Momentum Dispersion

In the first row of Figure 2, we note that the spin degeneracy of the system is lifted which is reflected in the graph as two distinct Dirac hyperbolas appear [10]. Similar results have been seen in previous models as the previously superposed Dirac cones in the surface states split in opposite directions in momentum space with opposite chirality, creating spin-polarized states [5,11].

The linear dispersion in the conduction (+) and valence band (-) that characterizes Dirac semimetals can be seen when there is no hybridization as seen in the graphs in the first row. However, as a result of the hybridization term, we see that the conduction and valence band take on a parabolic dispersion instead. We also note a drastic change in the band gap as it significantly increases due to the increase in hybridization as seen in the differences between the graphs with $\Delta_h = 0$ and $\Delta_h = 0.25$ [4].

3. Energy vs. Magnetic Field

After solving for the Landau levels of the Hamiltonian, we obtain the equality

$$E_{\alpha}(n) = t\sqrt{2ne\hbar^2 v_f^2 B + \mu_B^2 g^2 B^2 + \Delta_i^2 + 2\alpha\sqrt{\mu_B^2 g^2 B^2 \Delta_i^2 + \mu^2 g^2 B^2 \Delta_i^2 + 2\Delta_i^2 ne\hbar^2 v_f^2 B}} \quad (2)$$

for $n = 1, 2, 3, \dots$ and $E_{\alpha}(0) = \mu_B g^* B_0 + \alpha\sqrt{\Delta_i^2 + \Delta_h^2}$ for $n = 0$.

This shows that the energy for $n > 0$ is a function of \sqrt{B} , characteristic of ultrarelativistic Dirac fermions [9]. We also notice that the zeroth Landau level has a linear dependence to the magnetic field due to the Zeeman-type term. When we introduce the hybridization term

$\Delta_h = 0.25$, we see a distinct band gap especially at $B = 0$ T between the conduction and valence band, signifying gapped electronic transport, similar to what is seen in the energy-momentum dispersion.

We note that as the inversion asymmetry term increases, the Landau levels of the top and bottom surfaces become more offset in potential energy. This lifting of spin degeneracy caused by broken inversion symmetry can be experimentally measured by analyzing Shubnikov-de Haas (SdH) oscillations. Peaks in R_{xx} usually correspond to distinct Landau levels; however, due to broken inversion symmetry, we note that many Landau levels cross each other, especially when Δ_i is large. As a result, some peaks in R_{xx} could correspond to a different surface state instead of being a distinct Landau level. Experimentally, this has been seen in quantum-confined Cd_3As_2 where some extremas correspond to the same Landau level of a different surface state instead of a distinct Landau level [16]. We also note that as the Landau level index increases, the distance between peaks in R_{xx} also decreases, which can similarly be seen in the decrease in gaps between levels in Figure 3 [16]. Since Cd_3As_2 exhibits a 3D topological insulator-like state under quantum confinement, we could then compare it to the 3D topological insulator HgTe which has a narrow-gap and strong spin-orbit coupling similar to Cd_3As_2 [17]. Analysis of SdH oscillations in HgTe demonstrate that the Landau level crossings are

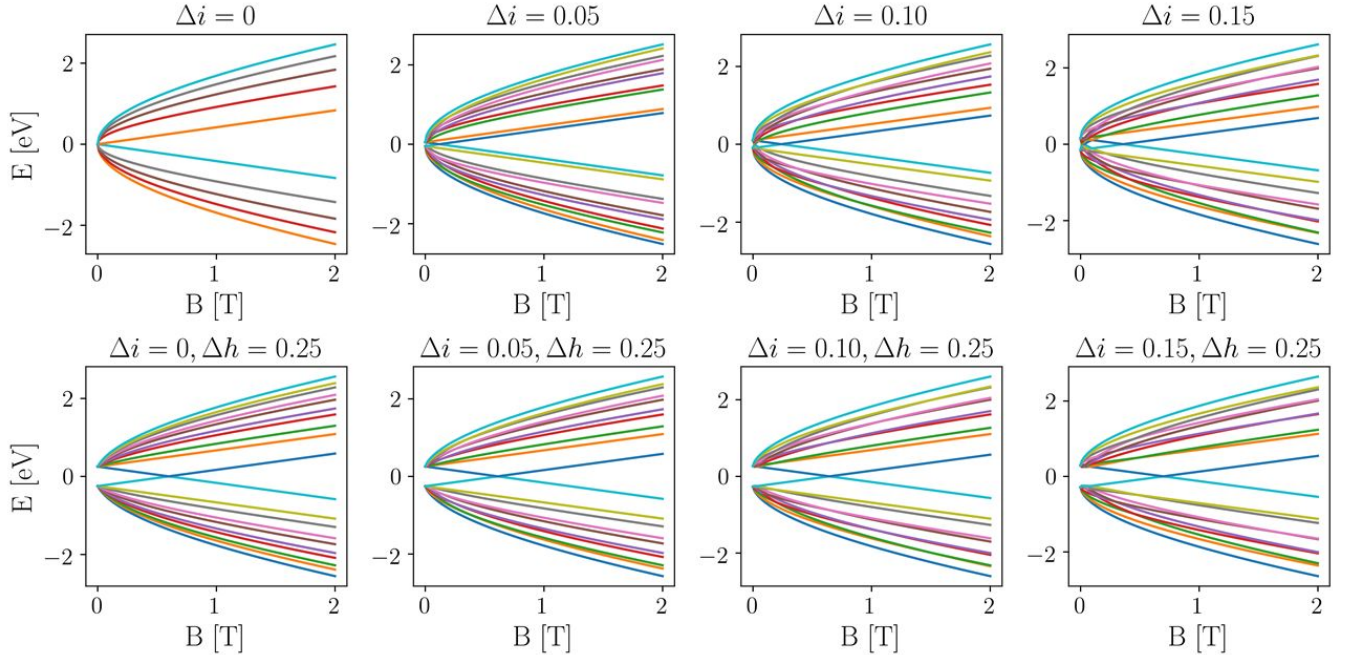


FIG. 3. First row: Energy vs. Magnetic Field with inversion asymmetry but no hybridization Second row: Energy vs. Magnetic Field with inversion asymmetry and hybridization

dominated by the structural inversion asymmetry as seen in the high Rashba S-O splitting energies [17]. Similar to experimental data on HgTe, our graphs also show that the crossing in Landau levels in Cd_3As_2 is due to inversion asymmetry since the number of crossings increase with increases in Δ_i . Another 3D topological insulator ($\text{Bi}_{1-x}\text{Sb}_x$) $_2\text{Te}_3$, which exhibits the half-integer Quantum Hall effect similar to Cd_3As_2 , showcases a lifted spin degeneracy due to structural inversion asymmetry as well [18]. Yoshimi *et al.* demonstrated that the Landau levels for the top and bottom surface corresponded to different energies, indicating that there was a difference in chemical potential, a source of inversion asymmetry [18]. Furthermore, while the top surface could fully form the $\nu = 1$ Quantum Hall state, the bottom surface could not fully form the $\nu = -1$ state, signifying a difference in energy between the top and bottom surfaces, indicative of inversion asymmetry.

4. Device Applications

We have shown that hybridization under quantum confinement creates a band gap at the Dirac point. With a significant band gap, the electronic transport of the system would stop if the Fermi-level is within that band gap. With this in mind, we could tune the Fermi-level to turn electronic transport on and off. Ziegler *et al.* have shown that one could tune the Fermi-level from the valence band to the conduction band through a top gate [12]. Thus, if the band gap was significant enough, the electronic transport would effectively be “off” and with

the application of an external electric field, the transport would be “on.” This could be extremely powerful in the creation of topological field effect transistors (Appendix 1) due to the quick response time and full electric control [13]. The application of an electric field, however, also breaks inversion symmetry, lifting spin-degeneracy and polarizing the electron spins in the surface states [11]. Dirac fermions in Cd_3As_2 have an extremely unique property which is its spin-momentum locking nature. Thus, by applying an electric field, one could lock the spin of the electrons in one direction and by reversing the current, lock the electrons in the opposite direction [14]. This manipulation of electron spin is desirable in spintronics devices such as SOT MRAM (Appendix 2) especially due to the high charge-spin conversion efficiency of Cd_3As_2 [15].

IV. CONCLUSIONS

Utilizing the Python package Kwant, we were able to characterize electronic interactions under quantum confinement with broken inversion symmetry and hybridization. We observed that broken inversion symmetry lifts spin degeneracy, creating spin-polarized states that could be utilized for spintronics applications such as SOT MRAM. We also demonstrated that through the band gap that is generated by hybridization, full electric control of electronic transport can be obtained through the tuning of the Fermi-level with an external electric field.

ACKNOWLEDGMENTS

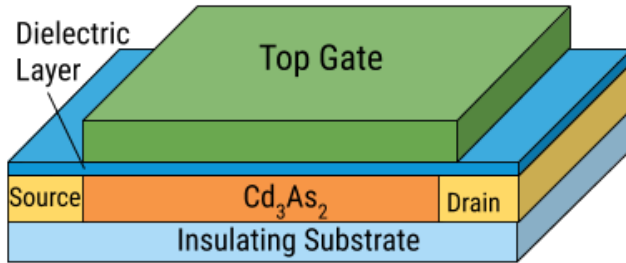
The first author would like to thank the second author for his expertise in condensed matter physics and his constant optimism and patience throughout the project. The first author also expresses gratitude for Dr. Lina Kim and T.A. Andrew McGrath for their support throughout the program.

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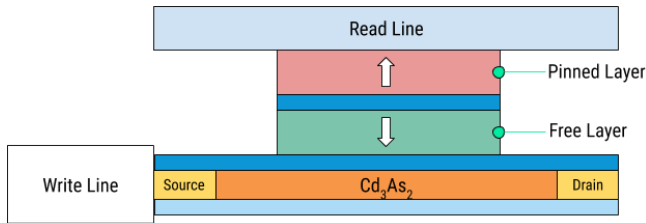
APPENDIX

1. Topological Field Effect Transistor



Example of a topological field effect transistor that can be controlled by an external electric field through the top gate. With the Fermi-level in the valence band, the electronic transport would be “off.” However, with the top gate, the Fermi-level could be tuned to the conduction band which turns on electronic transport.

2. Spin Orbit Torque MRAM



Example of a Spin Orbit Torque MRAM built with the Dirac semimetal Cd_3As_2 . With the application of an external electric field, the states in the surfaces of the thin film will become polarized, creating a torque that can change the orientation of the free layer. Then depending on the orientation of the electrons in the free layer, the resistance state would change which can be measured by the read line and can be recorded as a “0” or “1.”