First Principle Calculation of the Zeeman's Effect, Spin Zero Effect and Quantum Oscillation in Topological Materials

Dai Xi

Department of Physics

The Hong Kong University of Science and Technology

Email: daix@ust.hk

Abstract:
In this paper, we propose a first principle calculation method for the Zeeman's effect based on the second perturbation theory and apply it to a few topological materials. For Bi and Bi2Se3, our numerical results fit the experimental data quite well; for Na3Bi, TaN, and ZrTe5, the structure of the multi-bands Zeeman's couplings are derived from group theory and calculated by our method. Especially, we discussed the impact of Zeeman's coupling on the Fermi surface's topology in Na3Bi in detail. Finally, the spin zero angles for ZrTe5 was obtained from our calculation, which are in good agreement with the recent experimental results from XiaoSong Wu's group.