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Strong Correlation of Electron Saddle Point Singularities to the Anomalous Isotope Effect in Zr, Nb_3Sn, and $YBa_2Cu_3O_7$[1] GUANG-LIN ZHAO, Physics Department, Southern University and A&M College — Anomalously small isotope effect in some high and low T_c superconductors such as Zr, Nb_3Sn, and $YBa_2Cu_3O_7$ (YBCO) created a great challenge for understanding. It has been shown by experiments and first-principles calculations that there exist extended saddle point singularities in the electronic structures of these materials. In this work, a new methodology is further implemented by integrating first-principles calculations of electronic structures of the materials into the theory of many-body physics for superconductivity. The aim is to seek a unified methodology to calculate the electronic and superconducting properties of these materials. It is demonstrated from first-principles that the extended saddle point singularities in Zr, Nb_3Sn, and YBCO strongly correlate to the anomalous isotope effect in these superconductors. However, there still exist some differences between the calculated and experimental results that require further research work.

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