Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

First Principles Computation of G-Factors in Bi and Bi_2Se_3 ZHIDA SONG, SIMIN NIE, XI DI, ZHONG FANG, Chinese Academy of Sci (CAS), T03 TEAM — In this talk, we propose a first principles computation method for g-factor tensor,which not only gives comparable results with experiments but also establishes a clear physical picture of Zeeman effect in materials. In our method, the Hilbert space of the electronic states is treated as a direct product of "inner" space and "orbital" space, which are spanned by Bloch wave-functions and envelope functions respectively. Correspondingly, vector-potential is divided into a periodic part acting only in inner space and a non-periodic part acting only in orbital space. With the above flamework we define the g-factors as coupling coefficients between inner space and magnetic field. By the method we developed, we have further computed the g-factors of bismuth and Bi_2Se_3 and get satisfactory results, which are in good agreement with the experimental data.

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Date submitted: 27 Oct 2015 Electronic form version 1.4