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Indirect internuclear coupling in topological insulator Bi2Se3

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Topological insulators constitute a new class of material with an energy gap in the bulk and unusual metallic states on the surface. To date, most experiments have focused on probing the surface properties of these materials and suppressing the often inevitable contribution from bulk states. However, the bulk states in topological materials are of interest on their own and contain useful information that can be extracted with a local probe like nuclear magnetic resonance (NMR).

Recently, 77Se NMR experiments on Bi2Se3 single crystals have reported unusual field-independent linewidths and short spin-echo decays [1]. It is likely that an unexpectedly strong indirect internuclear coupling, characteristic of inverted band structures in topological materials, is the probable cause of these peculiar results.

The main objective of our research project is to provide a theory that explains the experiment of Ref. [1]. Starting from a microscopic tight-binding model for Bi2Se3, we calculate the Ruderman-Kittel-Kasuya-Yoshida (RKKY) and Bloembergen-Rowland (BR) couplings between nuclear spins, as well as the T1 relaxation time. We will compare our results to the experimentally available data.

[1] N. Georgieva, D. Rybicki, R. Guhne, G. Williams, S. Chong, I. Garate and J. Haase (arXiv: 1511.01727; manuscript submitted).

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