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Tight-binding theory of NMR shifts in topological insulators¹ ION GARATE, SAMUEL BOUTIN, Université de Sherbrooke, JORGE RAMIREZ RUIZ, Universidad Autónoma de México — To date, most experiments in topological insulators have focused on probing the surface states of these materials and suppressing the often inevitable contribution from bulk states. However, the latter 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 some inverted band structures, is the cause of these peculiar results. Motivated by this hypothesis, we report on a microscopic theory of NMR shifts and linewidths in Bi_2Se_3 and Bi_2Te_3 . Our theory provides quantitative estimates for the Knight shift, the orbital shift, the Ruderman-Kittel-Kasuya-Yoshida coupling and the Bloembergen-Rowland coupling. We will compare our findings with the available experimental data. [1] N. Georgieva, D. Rybicki, R. Guhne, G. Williams, S. Chong, I. Garate and J. Haase, arXiv:1511.01727 (2015)

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