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Calculation of diamagnetic susceptibility in Cu, graphite and Bi from band-structure[1] G. SAMOLYUK, J. SCHMALIAN, B. HARMON, S. BUD'KO, P. CANFIELD, AmesLab/Dept. of Physics, ISU — Since early pioneering work on the orbital diamagnetism of free electrons[1] the problem of calculation of diamagnetic susceptibility has attracted attention in systems such as graphite and bismuth. Recent interest in this problem has been motivated by the unconventional electronic properties of mono- and multilayered graphenes. These materials demonstrate large orbital diamagnetism caused by a specific type of band dispersion: a crossing of two bands, each with linear dispersion near the Fermi level. Significant progress in the theoretical description of orbital diamagnetism of electrons in periodic potentials was achieved by Fukuyama[2], with an exact expression for diamagnetic susceptibility, but with an approximation for band dispersion put in by hand. As an alternate approach, we use band structure obtained from a first-principles calculation (LMTO). The orbital susceptibility was calculated for Cu, as an example of a metal with small orbital diamagnetism, as well as for graphite and Bi, materials with known, large diamagnetic susceptibilities. [1] L. Landau, Z. Physik. **64**, (1930) 629. [2] H. Fukuyama, Prog. Theor. Phys. **45**, (1971) 704.

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