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Helmholtz Fermi surface harmonics: an efficient approach for treating anisotropic problems involving Fermi surface integrals ASIER EIGUREN, IDOIA G. GURTUBAY, Condensed Matter Physics. University of the Basque Country & Donostia International Physics Center (DIPC). — We present a new efficient numerical approach for representing an-isotropic physical quantities and/or matrix elements defined on the Fermi surface (FS) of metallic materials. The method introduces a set of numerically calculated generalized orthonormal functions, which are the solutions of the Helmholtz equation defined on the FS, where the periodicity of the reciprocal space is treated as a boundary condition. In essence, what we introduce is a generalization of the Spherical Harmonics for any periodic Fermi Surface and regardless of its topology. The main motivation of the approach is to handle an-isotropic many-body problems very efficiently. In this context we demonstrate how our theory reduces, by several orders of magnitude, the computational effort when applied to several well know many-body theoretical models such as the electron-phonon. Moreover, the method is demonstrated to be very robust in handling problems with any crystal structure or topology of the FS. We illustrate the method showing applications on several relevant surface and bulk systems.

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