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Abstract

Efficient Calculation of Anisotropic Fermi Surface Problems through Helmholtz Fermi Surface Harmonics †

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In metals, the details of the Fermi surface and the magnitude of the matrix elements connecting different points defined on it determine most of their transport properties, which are limited by the electron-phonon coupling and the scattering by impurities. Typically, the calculation of an anisotropic physical property defined on the Fermi surface, say in an impurity or Boltzmann transport problem, requires the consideration of several thousands of points on the surface. In contrast, the Helmholtz Fermi Surface Harmonics (HFSH) technique allows us to accurately treat these problems considering few elements of the HFSH set.

Here we introduce the recent developments we have implemented in this direction, including the symmetry treatment and the derived selection rules. We also show a representative benchmarking list of examples, illustrating the potential of this method.