Anisotropic Migdal–Eliashberg Calculations for MgB_2-Based Superconductors with Intermediate Representation and Ab-Initio Coulomb Interactions

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Keywords: Eliashberg calculations, Green's function, Electron-phonon coupling

Understanding the superconducting gap functions in MgB_2-based materials requires a quantitative treatment of both electron–phonon and Coulomb interactions. A quantitative description of phonon-mediated superconductors also provides an important benchmark for discussing pairing mechanisms in broader classes of superconducting materials. We have developed an efficient scheme for anisotropic Migdal–Eliashberg calculations by implementing the intermediate-representation (IR) basis [1] in the EPW code [2,3]. The IR basis makes it possible to include Matsubara frequencies up to the energy scale of Coulomb interactions even in Eliashberg calculations below 1 K, enabling estimates of the superconducting transition temperatures of simple metals such as aluminum [3]. However, our previous calculations did not fully account for the momentum dependence of the Coulomb interaction, which is essential for improving the predictive accuracy of transition temperatures and gap functions. In the present work, we incorporate screened Coulomb matrix elements obtained from GW calculations into anisotropic Migdal–Eliashberg calculations, thereby treating electron–phonon coupling and Coulomb repulsion on an equal footing. For MgB_2 and related compounds, the resulting superconducting gap functions and transition temperatures are consistent with experimental observations. We will discuss how anisotropic Coulomb interactions shape the multigap structure characteristic of MgB_2-type superconductors.

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