

Abstract Submitted
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The role of the Fermi surface sampling in first-principles calculations of electron-phonon coupling¹ FELICIANO GIUSTINO, MARVIN L. COHEN, STEVEN G. LOUIE, University of California at Berkeley — A quantitative understanding of the electron-phonon interaction is crucial to the understanding of conventional and possibly high- T_c superconductivity, as well as to the study of transport and spectroscopic (such as optical and photoemission) properties of bulk and nanoscale systems. Despite the enormous interest in calculating electron-phonon interaction from first principles, present methods carry severe practical limitations. We present here a comparative study of several existing methods for computing this quantity. We show that, independent of the approximation adopted, a common computational bottleneck is that the Fermi surface must be sampled with extremely high accuracy, leading to prohibitively expensive calculations for complex systems. We also reformulate the problem of evaluating phonon linewidths in terms of self-consistent linear response theory, and demonstrate our approach through application to magnesium diboride.

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