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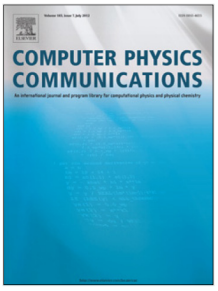

Efficient method to calculate the electron–phonon coupling constant and superconducting transition temperature

Takashi Koretsune, Ryotaro Arita

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Efficient method to calculate the electron-phonon coupling constant and superconducting transition temperature

Takashi Koretsune[a,b], Ryotaro Arita[a,c]

[a] *RIKEN, Center for Emergent Matter Science, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan*
[b] *JST, PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan*
[c] *ERATO Isobe Degenerate π-Integration Project, Tohoku University, Aoba-ku, Sendai 980-8578, Japan*

Abstract

We show an efficient way to compute the electron-phonon coupling constant, λ, and the superconducting transition temperature, T_c from first-principles calculations. This approach gives rapid convergence of T_c with respect to the size of the $\boldsymbol{k}$-point mesh, and is seamlessly connected to the formulation used in large molecular systems such as alkali fullerides where momentum dependence can be neglected. Since the phonon and electron-phonon calculations are time consuming particularly in complicated systems, the present approach will strongly reduce the computational cost, which facilitates high-throughput superconducting material design.

Keywords: first-principles calculation, electron-phonon coupling, superconductivity

1. Introduction

Precise prediction of the superconducting transition temperature, T_c, and designing high-temperature superconducting materials are one of the ultimate goals for material design. Particularly for phonon-mediated superconductivity, several recent studies based on superconducting density functional theory

*Corresponding author
Email address: takashi.koretsune@riken.jp (Takashi Koretsune)