عنوان مقاله:

Physical and mathematical justification of the numerical Brillouin zone integration of the Boltzmann rate equation by Gaussiansmearing

محل انتشار:

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نویسندگان:

Christian Iilg - *Max Planck Institute for Intelligent Systems, Heisenbergstr. ۳, ۷۰۵۶۹ Stuttgart, Germany*

Michael Haag - *Max Planck Institute for Intelligent Systems, Heisenbergstr. ۳, ۷۰۵۶۹ Stuttgart, Germany*

Nicolas Teeny - *Max Planck Institute for Nuclear Physics, Saupfercheckweg ۱, ۶۹۱۱۷ Heidelberg, Germany*

Jens Wirth - *Institut fu¨r Analysis, Dynamik und Modellierung, Universita¨t Stuttgart, Pfaffenwaldring ۵۷, ۷۰۵۶۹ Stuttgart, Germany*

خلاصه مقاله:

Scatterings of electrons at quasiparticles orphotons are very important for many topics in solid-statephysics, e.g., spintronics, magnonics or photonics, andtherefore a correct numerical treatment of these scatteringsis very important. For a quantum-mechanical description ofthese scatterings, Fermi's golden rule is used to calculatethe transition rate from an initial state to a final state in afirst-order time-dependent perturbation theory. One cancalculate the total transition rate from all initial states to allfinal states with Boltzmann rate equations involving Brillouinzone integrations. The numerical treatment of theseintegrations on a finite grid is often done via a replacementof the Dirac delta distribution by a Gaussian. The Diracdelta distribution appears in Fermi's golden rule where itdescribes the energy conservation among the interactingparticles. Since the Dirac delta distribution is a not afunction it is not clear from a mathematical point of viewthat this procedure is justified. We show with physical andmathematical arguments that this numerical procedure is ingeneral correct, and we comment on critical points.

کلمات کلیدی:

Electron scattering Boltzmann rate equations Brillouin zone integration Treatment of Diracs delta distribution