THE CHINESE UNIVERSITY OF HONG KONG

Department of Physics

SEMINAR

First-Principles Calculation of Magnetoresistance and Hall Effect in Real Materials

by

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Place: Rm G25, Science Centre North Block, CUHK

ALL INTERESTED ARE WELCOME
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Abstract

In this talk, we will introduce a nonperturbative first-principles methodology under magnetic fields, combined with semiclassical Boltzmann transport theory, to quantitatively compute magnetoresistance and the Hall effect in real materials. We discuss the unsaturated magnetoresistance observed in both top ologically trivial and nontrivial systems, revealing the critical roles of carrier compensation, open-orbit mechanisms, and Fermi-surface topology. Our theoretical predictions exhibit excellent agreement with low-temperature experimental data for prototypical metals, semimetals, Weyl semimetals, and magnetic materials. For the first time, we propose a scaling law governing Hall resistivity as a function of temperature and magnetic field. This new approach successfully explains the complex magnetoresistance and Hall-effect behaviors found in magnetic materials, aligning closely with experimental observations and underscoring the decisive influence of Fermi-surface geometry and the Lorentz force on magnetic transport properties. We also demonstrate that, under magnetic fields, the characteristic ρ – T curve no longer serves as a reliable criterion for distinguishing metals, semiconductors, or insulators. Our work provides a novel theoretical framework for understanding magnetic transport phenomena and introduces the WannierTools software for electronic-structure analysis, thereby opening new pathways for characterizing electronic structures.