Metal-insulator transition in disordered systems from the one-body density matrix

The insulating state of matter can be probed by means of a ground state geometrical marker, which is closely related to the modern theory of polarization (based on a Berry phase). In the present work we show that this marker can be applied to determine the metal-insulator transition in disordered systems. In particular, for noninteracting systems the geometrical marker can be obtained from the configurational average of the norm-squared one-body density matrix, which can be calculated within open as well as periodic boundary conditions. This is in sharp contrast to a classification based on the static conductivity, which is only sensible within periodic boundary conditions. We exemplify the method by considering a simple lattice model, known to have a metal-insulator transition as a function of the disorder strength, and demonstrate that the transition point can be obtained accurately from the one-body density matrix. The approach has a general ab initio formulation and could in principle be applied to realistic disordered materials by standard electronic structure methods.

General information
Publication status: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, University of Trieste, Universidad del Pais Vasco
Contributors: Olsen, T., Resta, R., Souza, I.
Number of pages: 6
Publication date: 2017
Peer-reviewed: Yes

Publication information
Journal: Physical Review B
Volume: 95
Issue number: 4
Article number: 045109
ISSN (Print): 2469-9950
Ratings:
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.149
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Original language: English
Electronic versions:
Untitled.pdf
DOIs:
10.1103/PhysRevB.95.045109

Bibliographical note
©2017 American Physical Society
Source: FindIt
Source-ID: 2350976413
Research output: Contribution to journal › Journal article – Annual report year: 2017 › Research › peer-review