Topological quantization and gauge-invariance of charge transport in liquid insulators

Federico Grasselli

SISSA – Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy

Charge transport is observed in electronically insulating fluids, such as molten salts, where the ionic diffusion leads to a non-vanishing static electrical conductivity even in the absence of conducting electrons. Standard tools to study the electric transport in such systems are provided by molecular dynamics (MD): according to the Green-Kubo theory of linear response [1], the electrical conductivity can be extracted from the time-correlation function of electric currents in equilibrium MD simulations. Despite the apparent simplicity of a naive classical description - where ions transport an integer, time independent, charge - in a first-principle framework the instantaneous electric currents are obtained from the Born effective charge tensors, which are real, tensor, and time-dependent quantities: a computationally time-consuming and conceptually abstruse task. Interestingly enough, if we aim at the static electrical conductivity, the same results are exactly obtained if the Born tensors are replaced by the integer oxidation numbers of the atoms [2]. We discuss how a recently-formulated gauge-invariance principle of transport coefficients [3], together with arguments from charge-transport quantization [4], can be employed to understand the latter unexpected coincidence, providing an alternative method to compute first-principle electrical conductivity of ionic fluids [5]. Examples and numerical experiments are given for the case of molten potassium chloride.

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