Charge transport in materials under external magnetic field

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Classical molecular dynamics simulations of ionic charge transport in condensed phase systems subject to an external magnetic field are surprisingly uncommon. This is due to two main difficulties. First, the non-canonical form of the Hamiltonian breaks standard time reversal invariance and key statistical relations do not hold in standard form. Second, the coupling between coordinates and momenta induced by the Lorentz force hinders straightforward application of common algorithms (e.g. velocity Verlet, Nose-Hoover thermostat) and of the periodic boundary conditions usually applied for bulk simulations.

Recent work [1,2,3,4] showing how these conceptual and practical difficulties can be circumvented will be presented in this talk. The application of these developments to charge transport in molten NaCl and in the superionic phase of AgI, with specific focus on detecting the possible on-set of the ionic Hall effect in these systems, will then be discussed [5,6].

[1] S. Bonella, G. Ciccotti and L. Rondoni, *European Physics Letter*, **108 60004 (2014)**

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[3] F. Mouhat, S. Bonella and C. Pierleoni, *Molecular Physics*, **111 3651 (2013)**

[4] A. Coretti, S. Bonella and G. Ciccotti, *The Journal of Chemical Physics Communications,* **149 191102 (2018)**

[5] L. Gagliardi, S. Bonella, *Physics Review B*, **94 134426 (2016)**

[6] D. Girardier, A. Coretti, G. Ciccotti, S. Bonella "Mass-Zero constrained dynamics and statistics for the shell model in magnetic field", **arXiv:2104.11650**