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# A tight-binding model for charge transport in silicate layers

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**Abstract**—Observations and experiments in silicates of the mica group show the transport of electric charge along the cation layers in absence of an electric field, a phenomenon called hyperconductivity. The transport of charge is achieved when a nonlinear vibration brings about that the ions become close enough for the transfer of an electron or hole. A model is developed in detail, approximations of different order for smaller vibration are considered so as to obtain approximate solutions. The full equations are integrated numerically with several approaches to overcome the problem caused by the different time scales of ion and electron movements. Localized solution showing the transport of charge coupled to nonlinear excitations are observed and described.

## Tight-binding model for charge transport along cation layers

Research from the sixties on the evidence of fossil tracks in mica produced by swift particles and nonlinear excitations was reviewed in Ref. [1]. The culmination of those eforta was the experimental demonstration of nonlinear excitations travelling along close-packed lines of an specimen of mica bombarded by alpha particles from one side and producing the ejection of an atom at the opposite side [2].

In the review it was realized and commented that only positive swift particles as positrons, antimuons and protons were producing dark tracks and that the source of energy for nonlinear excitations called quodons, the decay of $^{40}K$, also left behind an electric charge, which was positive in the 90% of cases. The hypothesis that dark tracks were produced by moving positive charge was proposed. It implied that quodons were carrying charge, mainly positive one [3].

Subsequently, the transport of electric charge by quodons produced by alpha bombardment in absence of an electric field was verified experimentally. It was called hyperconductivity [4, 5]. The phenomenon took place in several silicates of the mica group as muscovite, artificial or natural fluorphlogopite and lepidolite.

The bandgap of these insulators being extremely large implies that the conduction through carriers in the valence of conduction is not possible at room temperature. Charge transport takes place when large oscillations of the ions bring about the overlapping of the wavefunctions of two approaching ions and therefore allowing a finite probably of electron or hole transfer.

A tight-binding model for this phenomenon, where the ions are treated classically and the electron or hole as a quantum object is developed. Most of the parameters are known and recent theory on exact moving breathers [6] is adapted to tight-binding models.

An important problem is the large difference in the time scale of ions and electrons. There are several strategies to deal with the problem, particularly of interest are symplectic algorithms that conserve both the energy and electron wave function at each step.

We obtain localized solutions where the ion vibration and charge probability travel together. It is however difficult to achieve a long-life for those excitations as exact solutions are not easy to obtain due the different time scales. Several approaches are proposed to narrow the space of parameters based in physical properties of the materials studied.

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