Computational and physical problems for nonlinear charge transport in silicates

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Abstract—It has been shown that nonlinear waves can transport localized energy in silicates, both as neutral entities and carrying electric charge. The latter is of particular interest because it provides a magnitude to measure, the electric current. Models for charge transport in silicates and their properties are presented. They pose considerable computational and physical challenges.

1. Introduction

Hyperconductivity is the phenomenon of charge transport in absence of an electric field [1]. The energy and momentum is provided by the impact of swift particles or ion recoil after radioactive decay. Charge transport is mediated by solitary waves that bind to an electric charge.

Experiments on hyperconductivity have stimulated the study of exact solutions in Klein-Gordon systems in the form of travelling solitary waves through the spectral theory in the moving frame [2]. Those systems can allow for the description of charge transport by constructing a related semiclassical tight-binding system [3]

2. Results

For approximate phenomenological models, both exact breathers and polarobreathers are found [4]. For more realistic physical models a key magnitude is the transfer integral $\langle 1|\hat{H}_e|2\rangle$, where $|1\rangle = \Phi_1$ is the wave function of the electron at the ion K^+ at site 1 and $|2\rangle = \Phi_2$ at the nearest neighbour ion K^+ at site 2 and $\hat{H}_e$ is the electron Hamiltonian. It takes the functional form $I_0 = J_0 \exp(-\alpha(d_{n,n+1}))$ where $d_{n,n+1}$ is the distance between potassium ions in a silicate layer. Using the Slater approximation, we have been able to obtain the physical values of the transfer integral. These values introduce frequencies that are difficult to follow by integration methods.

For phenomenological models with constant on-site energy we have been able to obtain exact polarobreathers [4], but for realistic models the on-site energy depends on the Coulomb energy between a hole and an ion and changes considerably with large vibrations. There appear interesting solutions as chaobreathers, which provide a different form of localization coherent with the fact that the material is an insulator, but there are serious problems for energy propagation in a coherent way.

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References

[1] F.M. Russell, A.W. Russell, J.F.R. Archilla, EPL **127**(1), 16001 (2019)

[2] J.F.R. Archilla, Y. Doi, M. Kimura, Phys. Rev. E **100**(2), 022206 (2019)

[3] J.F.R. Archilla, J. Bajārs, Y. Doi, M. Kimura, J. Phys: Conf. Ser. (2024). To appear, arXiv:2308.1518

[4] J.F.R. Archilla, J. Bajārs, Axioms **12**(5), 437 (2023)