Spectrum of exact polarobreathers in tight-binding semiclassical systems

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Experiments have shown that alpha particles bring about the transport of charge at zero electric field across a few millimetres of layered silicates [1-4], a phenomenon called *hyperconductivity*. The current explanation is that the alpha particles produce nonlinear localized vibrations that bind to electrons or holes left behind by the beta decay of ^{40}K and that remains within the insulator. When this charge is exhausted the nonlinear vibrations can only transport the charge provided by the alpha particles as also observed experimentally. A semiclassical tight-binding model is appropriate to describe the experiments due to the large difference of the atoms and the electrons. Breathers, i.e., localized nonlinear vibrations have been shown to propagate in the model without charge [5]. When they couple to a charge they are known as polarobreathers. The problem of numerical integration without the Born-Oppenheimer approximation has been solved using splitting methods that are symplectic and conserve exactly the charge probability [6]. We present analytical and numerical analysis expanding the theory developed in [5,7] for systems with charge. It is of special interest the properties of the momentum-frequency spectrum of approximate and exact solutions that could be useful to identify these vibronic entities in spectroscopy.

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