Same polarity polaron and bipolaron scattering on conducting polymers

Maurício Bellissimo Falleiros^{1*} (PG), Geraldo Magela e Silva² (PQ)
mauricio.falleiros@ueg.br

¹ Goias State University, 75132-400, Anapolis/GO – Brazil,

currently at Institute of Physics – University of Brasília, 70.919-970, Brasília/DF – Brazil

² Institute of Physics – University of Brasília, 70.919-970, Brasília/DF – Brazil

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Abstract

Conducting polymers based technology has been evolving in several application fields, like opto-electronics, energy conversions and storage, sensors and actuators for mechanical and biological devices and others [1-6]. Detailed phenomenological comprehension of the dynamics of polarons and bipolarons, which are the charge carriers in these material, can improve the design and development of new applications.

Several studies has been carried out on the dynamics of scattering involving opposite charged quasi-particles [7-11], but we could not find any on quasi-particles with same sign charges. The present work addresses such situations in pristine chains of cis-polyacetylene and polyparaphenylene, both simple and prototypical polymers whose analysis is relatively easy and can shed light on more complex systems.

To accomplish this, we follow a systematic numerical investigation using a SSH Hamiltonian model extended to include intra-site and nearest neighbors electron-electron interactions, developed over a two dimensional hexagonal lattice [12].

We identify an intermediary range of relative velocities for which the polaron passes through the bipolaron, both keeping their integrity as a elemental charge multiple (e , $2e$) coupled to a distinct lattice deformation. Out of this range, an elastic or quasi-elastic collision takes place, as expected, and from this we can estimate the ratio between effective masses of polaron and bipolaron.

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