Quartic Lattice Interactions, Soliton-Like Excitations, and Electron Pairing in One-Dimensional Anharmonic Crystals

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In this study, it is shown that two added, excess electrons with opposite spins in one-dimensional crystal lattices with quartic anharmonicity may form a bisolectron, which is a localized bound state of the paired electrons to a soliton-like lattice deformation. It is also shown that when the Coulomb repulsion is included, the wave function of the bisolectron has two maxima, and such a state is stable in lattices with strong enough electron (phonon/soliton)–lattice coupling. Furthermore, the energy of the bisolectron is shown to be lower than the energy of the state with two separate, independent electrons, as even with account of the Coulomb repulsion the bisolectron binding energy is positive. © 2011 Wiley Periodicals, Inc.

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Introduction

In a previous publication,[1] we have considered soliton-mediated electron pairing in anharmonic lattices endowed with cubic interparticle interaction. The latter is of mathematical interest, as it underlies as a dynamical system the soliton-bearing Boussinesq–Korteweg-de Vries equation governing wave propagation along the lattice in the continuum approximation.[2–4] Noteworthy is that due to the electron–lattice interaction, the soliton arising from the cubic interaction is able to trap an electron, thus, leading to a solectron[5–7] in a way that generalizes the polaron concept long ago proposed by Landau and Pekar to describe electron self-trapping leading to a dressed electron (or, more generally, a quasiparticle).[8–11] In Ref. [1], it was shown that when two excess electrons are added the corresponding electron–lattice interaction also facilitates electron pairing leading to a bisolectron, that is, the localized bound state of the paired electrons and a soliton-like lattice deformation (otherwise said strongly correlated electrons in real space and momentum space). Here, we study this problem for a lattice with the apparently more physically appealing quartic particle interaction.

In Hamiltonian and Evolution Equations section, we pose the problem, introduce the Hamiltonian and the evolution equations of the system. Localized Solutions section is devoted to the search of localized, soliton-like traveling solutions. Then, in Energy of the Bisolectron and Role of the Coulomb Repulsion section, we asses the role of repulsive Coulomb interaction between the two added, excess electrons, satisfying Pauli's exclusion principle. Finally, in Conclusions section, we briefly recall the major results found.

Hamiltonian and Evolution Equations

We consider a one-dimensional (1D) model, infinitely long crystal lattice with electrons and lattice particles of equal masses M, describable by the following Hamiltonian:[10,11]

$$\hat{H} = \hat{H}_{el} + \hat{H}_{lat} + \hat{H}_{int}, \tag{1}$$

with

$$\hat{H}_{el} = \sum_{n,s} [E_0 \hat{B}^+_{n,s} \hat{B}_{n,s} - J\hat{B}^+_{n,s}(\hat{B}_{n+1,s} + \hat{B}_{n-1,s})], \tag{2}$$

$$\hat{H}_{lat} = \sum_{n} \left[\frac{\hat{p}_n^2}{2M} + \hat{U}\right], \tag{3}$$

$$\hat{H}_{int} = \chi \sum_{n,s} (\hat{\beta}_{n+1} - \hat{\beta}_{n-1})\, \hat{B}^+_{n,s}\hat{B}_{n,s}. \tag{4}$$

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