Electron Pairing in One-Dimensional Anharmonic Crystal Lattices

M. G. VELARDE,[1] L. BRIZHIK,[1,2] A. P. CHETVERIKOV,[1,3] L. CRUZEIRO,[1,4] W. EBELING,[1,5] G. RÖPKE[1,6]

[1]*Instituto Pluridisciplinar, Universidad Complutense, Paseo Juan XXIII, 1, Madrid 28040, Spain*
[2]*Bogolyubov Institute for Theoretical Physics, Metrolohichna Str., 14b, Kyiv 03680, Ukraine*
[3]*Faculty of Physics, Chernyshevsky State University, Astracanskaya 83, Saratov 410012, Russia*
[4]*CCMAR and FCT, Universidade do Algarve, Portugal, Campus de Gambelas, Faro 8005-139, Portugal*
[5]*Institut für Physik, Humboldt Universität, Newtonstrasse 15, Berlin 12489, Germany*
[6]*Institut für Physik, Universität Rostock, Universitätsplatz, 3, Rostock 18051, Germany*

Received 9 September 2010; accepted 15 November 2010
Published online 8 March 2011 in Wiley Online Library (wileyonlinelibrary.com).
DOI 10.1002/qua.23008

ABSTRACT: We show that when anharmonicity is added to the electron–phonon interaction it facilitates electron pairing in a localized state. Such localized state appears as singlet state of two electrons bound with the traveling local lattice soliton distortion, which survives when Coulomb repulsion is included. ©2011 Wiley Periodicals, Inc. Int J Quantum Chem 112: 551–565, 2012

Key words: anharmonic lattice; lattice soliton; solectron; electron pairing; bisolectron

1. Introduction

It is known that the electron–phonon interaction results in the lowering of the energy of quasi-particles (dressed electrons, holes, excitons, etc.) [1–6]. Depending on the strength of the coupling and the ratio between the Debye energy of phonons and the characteristic energy of a quasi-particle (band width), the latter is either in an almost free band state or is trapped in a large polaron or small polaron state [1–6]. For instance, at moderate values of coupling, large polarons correspond to the lowest energy of the system [6]. From the point of view of conducting properties, the large polaron is the most important case, and there is a wide class of crystals where the necessary conditions for its formation are fulfilled. In one-dimensional (1D) molecular crystals, such large polarons have been described by soliton-bearing nonlinear evolution equations and are

Correspondence to: M. G. Velarde; e-mail: mgvelarde@pluri.ucm.es

Contract grant sponsor: Spanish Ministerio de Ciencia e Innovación.
Contract grant number: EXPLORA-FIS2009-06585-E.
Contract grant sponsor: Fundamental Research Grant of the National Academy of Sciences of Ukraine.
Contract grant sponsor: Ministry of Education and Science of the Russian Federation.
Contract grant number: 14.740.11.0074.
Contract grant sponsor: Portuguese Fundação para a Ciência e Tecnologia.