



VI International Symposium on
**Strong Nonlinear Vibronic and
Electronic Interactions in Solids**

BOOK OF ABSTRACTS

NONLINEAR DYNAMICS OF CRYSTAL LATTICES
STRONGLY CORRELATED ELECTRONIC SYSTEMS
SOLID STATE SPECTROSCOPY
NONLINEAR QUANTUM OPTICS

April 28 – May 1, 2018
Tartu, Estonia

Book of abstracts of the "VI International Symposium on Strong Nonlinear Vibronic and Electronic Interactions in Solids"

April 28 - May 1, 2018, Tartu, Estonia

Edited by V. Boltrushko

<http://ttl.ut.ee/ws18/book-of-abstracts.pdf>

This work has been supported by

- Institute of Physics, University of Tartu, Estonia
- Max Planck Institute for Solid State Research, Stuttgart, Germany
- Brandenburg University of Technology, Cottbus, Germany
- Tartu City Government, Tartu, Estonia



Organizing Committee

- **Vladimir Hizhnyakov** (Institute of Physics, University of Tartu, Estonia)
- **Reinhard K. Kremer** (Max Planck Institute, Stuttgart, Germany)
- **Götz Seibold** (Brandenburg Technical University, Cottbus, Germany)

Preface

Over the past decades an intense collaboration between Estonian and German researchers has developed in the field of condensed matter physics, reflected by the organization of a series of bilateral Estonian-German workshops in 2008, 2009, and 2011. From 2013 the bilateral format of the meetings has developed into an international scientific workshop on current topics in condensed matter physics and a special focus on nonlinear phenomena. In order to keep the workshop compact and its topics focused on the chosen problems, it is supposed that the number of participants will be limited and the participants will have to be invited/approved by the Organizing Committee.

We note that established close collaboration of German and Estonian scientists has an historical background: Adolf von Harnack - the founder and the first President of Kaiser-Wilhelm-Gesellschaft zur Förderung der Wissenschaften (now Max-Planck-Gesellschaft) was born in Tartu and graduated from Dorpat (at present Tartu) University.

Topics of the workshop include nonlinear dynamics of crystal lattices, strongly correlated electronic and magnetic systems, solid state spectroscopy and nonlinear quantum optics.

Practical Hints

All lectures are held in the Dorpat Conference Centre (on the 4th floor of the Tasku Centre in Turu 2) and in the Institute of Physics (W. Ostwaldi Str 1). The registration and sessions will take place in the Peterson Hall of the Conference Centre. Coffee breaks will be organized near the lecture rooms.

The duration of oral presentation is set to 22 min plus 3 min for discussion. We wish to avoid the use of participants' laptops for presentation that usually leads to a waste of time. Rather hand a flash with the file of your presentation to organizers. This can be done during the coffee break before your talk. The file will be copied on our laptop connected to an LCD projector. Types for the presentation files are MS PowerPoint and Adobe Acrobat, the latter is preferable. In the lecture hall, there will be also a whiteboard with color markers.

Stands for poster presentations are of A0 format. Posters can be fastened to them by paper-clips, which will be provided by organizers.

Wireless internet access is available in the conference rooms.

Programme

Saturday, April 28

- 18:00 – 19:00 Excursion in Tartu
(begins at 18:00 from the central square (Raekoja plats), near the statue of Kissing Students)
- 19:00 – 21:00 Welcome reception, early registration
(at University Café, Ülikooli 20)

Sunday, April 29, Dorpat Conference Centre, Turu 2

- 08:30 – 09:00 Registration
- 09:00 – 09:20 Opening ceremony
- 1st Session: Lattice Dynamics**
- 09:20 – 10:00 A.J. Sievers
Intrinsic localized modes in nonlinear lattices with applications
- 10:00 – 10:25 B. Tsukerblat
A symmetry assisted approach to multidimensional vibronic problem: theoretical background and applications
- 10:25 – 10:50 A. Bussmann-Holder
What makes the difference in perovskite titanates?
- 10:50 – 11:10 *Coffee break*
- 2nd Session: Strong Correlations**
- 11:10 – 11:35 K.I. Kugel
Half-metallic states in a doped density-wave insulator
- 11:35 – 12:00 G. Seibold
Spin-charge conversion at oxide interfaces
- 12:00 – 12:25 D.M. Dzebisashvili
London penetration depth in the ensemble of spin-polarons of cuprate superconductors
- 12:25 – 12:50 J. Röhler
Underdoped/Overdoped symmetry of cuprate superconductors
- 12:50 – 14:00 *Lunch*

3rd Session: Electron-Lattice Interactions

- 14:00 – 14:25 N.N. Rosanov
1D-, 2D-, and 3D-topological laser solitons
- 14:25 – 14:50 I.A. Shepelev
Investigation of subsonic crowdion induced mass transfer in metals
- 14:50 – 15:15 K. Noatschk
Monte Carlo simulations of Sn induced defects on the Ge(001) surface reconstruction
- 15:15 – 15:40 A. Möller
Canted screw-type motion and dynamics of the electronic ground state in low dimensional Fe(II) compounds
- 15:40 – 16:00 *Coffee break*

4th Session: Magnetic Excitations

- 16:00 – 16:25 A.V. Mikheyenkov
Isotropic helical states in frustrated magnetism: continuous transitions on the J_1 - J_2 - J_3 globe
- 16:25 – 16:50 E.A. Karatsuba
The inversion probability of a large spin as an asymptotic expansion in series of Bessel functions
- 16:50 – 17:15 Y. Zolotaryuk
Nonlinear excitations in arrays of magnetic dots
- 17:15 – 17:40 A.A. Tsirlin
Spin liquid and dimerization in the Kitaev hyperhoneycomb magnet β -Li₂IrO₃

5th Session: Posters (17:40 – 19:00)

- P01 P. Rubin
Spin-1/2 Heisenberg model on one-third-depleted square lattice: exact diagonalization study
- P02 V. Hizhnyakov, H. Kaasik, K. Pae
Dynamical Jahn-Teller effect: time evolution of vibronic states in conical intersection
- P03 A. Pishtshev, P. Rubin
Substitution effects in FeAs_2 : a route to advanced materials
- P04 D. Nevedrov
Predictive modeling with *TensorFlow*
- P05 I. Rebane
Time dependent (transient) theory of resonant secondary emission at two-step absorption of two light pulses
- P06 V. Hizhnyakov, K. Kugel, I. Tehver
Tunneling in resonance Raman scattering
- P07 A. Loot, V. Hizhnyakov
Spontaneous parametric-down conversion in plasmonic structures
- P08 A. Golubev, R.E. Dinnebier, A. Schulz, R.K. Kremer, H. Langbein, A. Senyshyn, J.M. Law, T. Hansen, H.-J. Koo, M.-H. Whangbo
Magnetic and Structural Properties of the Trirutile-type 1D Heisenberg Antiferromagnet CuTa_2O_6
- P09 V. Hizhnyakov
Supersonic solitons in Fermi-Pasta-Ulam chain
- P10 K. Pae, V. Hizhnyakov
Origin of ground state of $E \otimes e$ Jahn-Teller system
- P11 G. Litak, T. Örd, K. Rågo, A. Vargunin
Two-orbital superconductor with anisotropic pairing: characteristic lengths
- P12 T. Örd, K. Rågo, A. Vargunin, G. Litak
On the temperature behavior of Cooper pairs sizes in a two-band superconductor
- P13 V. Boltrushko, V. Hizhnyakov
Anomalous temperature dependence of vibronic spectra in low-dimensional systems
- P14 A. Shelkan, M. Klopov, V. Hizhnyakov
Supermobile small size solitons in a monatomic chain with odd anharmonicity
- P15 P. Konsin, B. Sorkin
Theory of superconducting surfaces and electrostatic doping dependence of critical temperature of high- T_c cuprate ultrathin films in the transverse electric field
- P16 V. Hizhnyakov
Intrinsic localized modes in two atomic chains; reduction of cubic anharmonicity for gap modes

Monday, April 30, Institute of Physics, W. Ostwaldi 1

08:30 – 09:00 Bus from hotels to the Institute of Physics

6th Session: Electron-Lattice Interactions

09:00 – 09:25 A.M. Oleś
Spin-orbital model of stoichiometric LaMnO_3 with tetragonal distortions

09:25 – 09:50 P. Lemmens
Phonons probe topological degrees of freedom in Dirac and Weyl semimetals

09:50 – 10:15 R. Stern
NMR investigation of the frustrated spin chain compound $\beta\text{-TeVO}_4$

10:15 – 10:40 N. Kovaleva
Multi-order Raman scattering in orthorhombic manganites

10:40 – 11:00 *Coffee break*

11:00 – 11:30 Familiarization with the Institute of Physics

7th Session: Lattice Dynamics

11:30 – 11:55 F. Piazza
Transient localization of gap modes in crystals of NaI at high temperature: insight and questions from wavelet analysis

11:55 – 12:20 E.A. Korznikova
Delocalized vibrational modes in graphene: second harmonic generation and negative pressure

12:20 – 12:45 S.V. Dmitriev
Effect of discrete breathers on energy transport in 1D nonlinear lattices

12:45 – 14:00 *Lunch*

8th Session: Superconductivity

14:00 – 14:25 M. Silaev
Spontaneous currents in spatially inhomogeneous $s + is$ superconductors

14:25 – 14:50 A.M. Gabovich
Quasiparticle current-voltage characteristics for break junctions involving d -wave superconductors unstable against charge-density-wave formation

14:50 – 15:10 Bus from the Institute to the excursion

15:10 – 17:00 Excursion to the Estonian National Museum

17:00 – 17:20 Bus to the hotel Dorpat

19:00 – 22:00 *Dinner* in the restaurant of the hotel Dorpat

Tuesday, May 1, Dorpat Conference Centre, Turu 2

9th Session: Lattice Dynamics

- 09:00 – 09:25 G. Chechin
Nonlinear atomic vibrations in strained graphene monolayer: bushes of nonlinear normal modes
- 09:25 – 09:50 J.F.R. Archilla
Nonlocal breathers as possible energy carriers in secondary tracks in muscovite
- 09:50 – 10:15 Yu.A. Kosevich
Phase dynamics of nonlinear localized excitations in weakly coupled anharmonic chains and analogy between periodic tunneling of classical and quantum objects
- 10:15 – 10:40 V. Dubinko
Discrete breathers in hydrogenated metals: atomistic simulations and applications to the rate theory
- 10:40 – 11:00 *Coffee break*

10th Session: Strong Correlations

- 11:00 – 11:25 C. Janowitz
Out of plane s -orbital contributions investigated by resonant photoemission on (Bi, Pb)₂201 and (Bi, Pb)₂212
- 11:25 – 11:50 A. Sherman
Influence of spin and charge fluctuations on spectra of the two-dimensional Hubbard model
- 11:50 – 12:15 V.I. Kuz'min
Influence of short-range correlations on the band structure of doped Mott insulators
- 12:15 – 14:00 *Lunch*

11th Session: Strong Correlations and ab initio calculations

- 14:00 – 14:25 N.M. Chtchelkatchev
Boson magnetism in strongly correlated cold atom system
- 14:25 – 14:50 M.M. Korovushkin
Stability of the superconducting d-wave pairing towards the Coulomb repulsions in cuprate superconductors
- 14:50 – 15:15 E. Strugovshchikov
Effects of chirality and strong electron localization in a crystalline yttrium oxyhydride
- 15:15 – 15:40 V. Krasnenko
The similarity of vibronic mechanisms during dimerization and reverse recovery of the aromatic compounds
- 15:40 – 16:00 *Coffee break*

12th Session: Superconductivity and Lattice Dynamics

- 16:00 – 16:25 A.P. Chetverikov
Dynamics of paired electrons and holes in bilayer nonlinear lattices and transport of the pairs by soliton-like excitations
- 16:25 – 16:50 A. Vargunin
Flux-flow spin Hall effect in type-II superconductors
- 16:50 – 17:15 O. Usoltsev
Nonlinear atomic vibrations and structural phase transitions in strained carbon chains
- 17:15 – 17:25 **Closing**

Table of Contents

Oral presentations

Day 1

<i>Intrinsic localized modes in nonlinear lattices with applications</i> A.J. Sievers	1
<i>A symmetry assisted approach to multidimensional vibronic problem: theoretical background and some applications</i> B. Tsukerblat	2
<i>What makes the difference in perovskite titanates?</i> A. Bussmann-Holder	3
<i>Half-metallic states in a doped density-wave insulator</i> K.I. Kugel	4
<i>Spin-charge conversion at oxide interfaces</i> G. Seibold	5
<i>London penetration depth in the ensemble of spin-polarons of cuprate superconductors</i> D.M. Dzebisashvili	6
<i>Underdoped/Overdoped symmetry of cuprate superconductors</i> J. Röhler	7
<i>1D-, 2D-, and 3D-topological laser solitons</i> N.N. Rosanov	8
<i>Investigation of subsonic crowdion induced mass transfer in metals</i> I.A. Shepelev	9
<i>Monte Carlo simulations of Sn induced defects on the Ge(001) surface reconstruction</i> K. Noatschk	10
<i>Canted screw-type motion and dynamics of the electronic ground state in low dimensional Fe(II) compounds</i> A. Möller	11
<i>Isotropic helical states in frustrated magnetism: continuous transitions on the J_1-J_2-J_3 globe</i> A.V. Mikheyenkov	12

<i>The inversion probability of a large spin as an asymptotic expansion in series of Bessel functions</i>	
E.A. Karatsuba	13

<i>Nonlinear excitations in arrays of magnetic dots</i>	
Y. Zolotaryuk	14

<i>Spin liquid and dimerization in the Kitaev hyperhoneycomb magnet β-Li₂IrO₃</i>	
A.A. Tsirlin	15

Day 2

<i>Spin-orbital model of stoichiometric LaMnO₃ with tetragonal distortions</i>	
A.M. Oleś	16

<i>Phonons probe topological degrees of freedom in Dirac and Weyl semimetals)</i>	
P. Lemmens	17

<i>NMR investigation of the frustrated spin chain compound β-TeVO₄</i>	
R. Stern	18

<i>Multi-order Raman scattering in orthorhombic manganites</i>	
N. Kovaleva	19

<i>Transient localization of gap modes in crystals of NaI at high temperature: insight and questions from wavelet analysis</i>	
F. Piazza	20

<i>Delocalized vibrational modes in graphene: second harmonic generation and negative pressure</i>	
E.A. Korznikova	21

<i>Effect of discrete breathers on energy transport in 1D nonlinear lattices</i>	
S.V. Dmitriev	22

<i>Spontaneous currents in spatially inhomogeneous $s + is$ superconductors</i>	
M. Silaev	23

<i>Quasiparticle current-voltage characteristics for break junctions involving d-wave superconductors unstable against charge-density-wave formation</i>	
A.M. Gabovich	24

Day 3

<i>Nonlinear atomic vibrations in strained graphene monolayer: bushes of nonlinear normal modes</i>	
G. Chechin	25

<i>Nonlocal breathers as possible energy carriers in secondary tracks in muscovite</i> J.F.R. Archilla	26
<i>Phase dynamics of nonlinear localized excitations in weakly coupled anharmonic chains and analogy between periodic tunneling of classical and quantum objects</i> Yu.A. Kosevich	27
<i>Discrete breathers in hydrogenated metals: atomistic simulations and applications to the rate theory</i> V. Dubinko	28
<i>Out of plane s-orbital contributions investigated by resonant photoemission on (Bi, Pb)₂201 and (Bi, Pb)₂212</i> C. Janowitz	29
<i>Influence of spin and charge fluctuations on spectra of the two-dimensional Hubbard model</i> A. Sherman	30
<i>Influence of short-range correlations on the band structure of doped Mott insulators</i> V.I. Kuz'min	31
<i>Boson magnetism in strongly correlated cold atom system</i> N.M. Chtchelkatchev	32
<i>Stability of the superconducting d-wave pairing towards the Coulomb repulsions in cuprate superconductors</i> M.M. Korovushkin	33
<i>Effects of chirality and strong electron localization in a crystalline yttrium oxyhydride</i> E. Strugovshchikov	34
<i>The similarity of vibronic mechanisms during dimerization and reverse recovery of the aromatic compounds</i> V. Krasnenko	35
<i>Dynamics of paired electrons and holes in bilayer nonlinear lattices and transport of the pairs by soliton-like excitations</i> A.P. Chetverikov	36
<i>Flux-flow spin Hall effect in type-II superconductors</i> A. Vargunin	37
<i>Nonlinear atomic vibrations and structural phase transitions in strained carbon chains</i> O. Usoltsev	38

Posters

<i>Spin-1/2 Heisenberg model on one-third-depleted square lattice: exact diagonalization study</i> P. Rubin	39
<i>Dynamical Jahn-Teller effect: time evolution of vibronic states in conical intersection</i> V. Hizhnyakov, H. Kaasik, K. Pae	40
<i>Substitution effects in FeAs₂: a route to advanced materials</i> A. Pishtshev, P. Rubin	41
<i>Predictive modeling with TensorFlow</i> D. Nevedrov	42
<i>Time dependent (transient) theory of resonant secondary emission at two-step absorption of two light pulses</i> I. Rebane	43
<i>Tunneling in resonance Raman scattering</i> V. Hizhnyakov, K. Kugel, I. Tehver	44
<i>Spontaneous parametric-down conversion in plasmonic structures</i> A. Loot, V. Hizhnyakov	45
<i>Magnetic and Structural Properties of the Trirutile-type 1D Heisenberg Antiferromagnet CuTa₂O₆</i> A. Golubev, et al.	46
<i>Supersonic solitons in Fermi-Pasta-Ulam chain</i> V. Hizhnyakov	47
<i>Origin of ground state of $E \otimes e$ Jahn-Teller system</i> K. Pae, V. Hizhnyakov	48
<i>Two-orbital superconductor with anisotropic pairing: characteristic lengths</i> G. Litak, T. Örd, K. Rågo, A. Vargunin	49
<i>On the temperature behavior of Cooper pairs sizes in a two-band superconductor</i> T. Örd, K. Rågo, A. Vargunin, G. Litak	50
<i>Anomalous temperature dependence of vibronic spectra in low-dimensional systems</i> V. Boltrushko, V. Hizhnyakov	51
<i>Supermobile small size solitons in a monatomic chain with odd anharmonicity</i> A. Shelkan, M. Klopov, V. Hizhnyakov	52
<i>Theory of superconducting surfaces and electrostatic doping dependence of critical temperature of high-T_c cuprate ultrathin films in the transverse electric field</i> P. Konsin, B. Sorkin	53
<i>Intrinsic localized modes in two atomic chains; reduction of cubic anharmonicity for gap modes</i> V. Hizhnyakov	54

Intrinsic localized modes in nonlinear lattices with applications

A.J. Sievers*¹

¹*Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY 14850, USA*

Impurity vibrational modes in crystals were predicted by I.M. Lifshitz in 1945 and first observed by G. Schaefer in 1960. It was soon discovered that the spectra of defective crystals contained an abundance of linear local vibrational modes outside of the standard phonon spectral range. More than a score of years passed before it was proposed that increased vibrational energy content in a nonlinear crystal lattice could appear as an intrinsic localized mode above the phonon spectrum, with its spatial extent only ranging over a very few lattice sites. The energy profiles of these intrinsic localized modes resemble those of impurity localized vibrational modes at defects in a harmonic lattice but, like solitons, they can propagate; however, in contrast with solitons they lose energy as they move through the lattice - the more localized the excitation the faster the energy loss. The theoretical behavior of these intrinsic localized modes has developed rapidly and evolved in three main directions: (1) to discover the properties of highly-localized large-amplitude excitations, (2) to assess their importance for real solids and (3) to determine the general behavior of discrete nonlinear systems, with emphasis on identifying soliton-like behavior. A variety of experiments quantifying such intrinsic localized modes followed and the experiments to be described here deal both with microscopic localized magnetic excitations and also with different kinds of macroscopic excitations in nonlinear transmission lines.

*Corresponding author: ajs19@cornell.edu

A symmetry assisted approach to multidimensional vibronic problem: theoretical background and some applications

Boris Tsukerblat^{*1}, Andrew Palii^{2,3}, Juan M. Clemente-Juan⁴, and Eugenio Coronado⁴

¹*Ben-Gurion University of the Negev, Department of Chemistry, Beer-Sheva, Israel*

²*Institute of Problems of Chemical Physics, Chernogolovka, Moscow Region, Russia*

³*Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau, Moldova*

⁴*Instituto de Ciencia Molecular, Universidad de Valencia, Polígono de la Coma, s/n, 46980 Paterna, Spain*

The classical treatment of the nuclear motion is invalid (despite the difference in masses of electrons and nuclei) in the region of crossover of the electronic terms or, more commonly, when we are dealing with the orbitally degenerate or pseudo degenerate levels. To overcome significant limitations implied by the adiabatic approach, we proposed a symmetry-adapted approach [1,2] combined with the efficient program VIBPACK [3] aimed to the accurate solution of the quantum-mechanical (dynamic) vibronic problem in large scale systems. The systems under consideration are supposed to consist of a set of electronic levels mixed by the active Jahn-Teller (JT) and pseudo JT vibrational modes. The algorithm for the solution of the eigen-problem takes full advantage of the point symmetry arguments. Applying the successive coupling of the bosonic creation operators, we introduce the irreducible tensors that can be referred to as multivibronic operators. Action of the irreducible multivibronic operators on the vacuum state creates the vibrational symmetry adapted basis that is subjected to the Gram-Schmidt orthogonalization at each step of evaluation. Finally, the generated vibrational basis is coupled to the electronic one to get the symmetry adapted electron-vibrational (vibronic) basis within which the full matrix of the JT Hamiltonian is blocked according to the irreducible representations of the point group. The proposed approach allows to treat optical and thermodynamic properties of large (nanoscale) multilevel system coupled to degenerate vibrations such as multispin systems and impurity centres in crystals. We illustrate in detail the developed technique by the application to molecular systems, such as $2e$ -reduced MV dodecanuclear Keggin anion in which the electronic pair is delocalized over twelve sites. VIBPACK together with the previously reported MAGPACK and MVPACK represent the full set of the theoretical tools to treat the nanoscale systems with the localised and itinerant spins within the frame of parametric effective Hamiltonian approach.

Acknowledgements: B.T. thanks University of Valencia for the Sabbatical Grant (Estades Temporals Investigadors Convidats). A.P., B.T. and J.M.C.J. acknowledge support from the Ministry of Education and Science of Russian Federation (Agreement No.14.W03.31.0001-Institute of Problems of Chemical Physics of RAS, Chernogolovka). The present work has been supported by the EU (COST Action CA15128 Molecular Spintronics (MOLSPIN)), the Spanish MINECO (CTQ2014-52758-P, MAT2014-56143-R and Excellence Unit María de Maeztu, MDM-2015-0538) and Generalitat Valenciana (Prometeo and ISIC Programmes of Excellence).

- [1] B. Tsukerblat, A. Palii, J.M. Clemente-Juan, A. Gaita-Ariño, E. Coronado, A symmetry adapted approach to the dynamic Jahn-Teller problem: application to mixed-valence polyoxometalate clusters with Keggin structure, *Int. J. Quantum Chemistry* **112**, 2957-2964 (2012).
- [2] J.M. Clemente-Juan, A. Palii, E. Coronado, B. Tsukerblat, Mixed-valence molecular unit for quantum cellular automata: beyond the Born-Oppenheimer paradigm through the symmetry assisted vibronic approach *J. Chem. Theory. Comp.* **12**, 3545-356 (2016).
- [3] J.M. Clemente-Juan, A. Palii, B. Tsukerblat, E. Coronado, VIBPACK: A Package to Treat Multidimensional electron-vibrational molecular problems with application to magnetic and optical properties, *Comp. Chemistry*, in press.

*Corresponding author: tsuker@bgu.ac.il

What makes the difference in perovskite titanates?

Annette Bussmann-Holder*¹, Krystian Roleder², and Jae-Hyeon Ko³

¹Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany

²Institute of Physics, University of Silesia, ul. Uniwersytecka 4, PL-40-007 Katowice, Poland

³Department of Physics, Hallym University, Chuncheon, Gangwondo 24252, Korea

We have investigated in detail the lattice dynamics of five different perovskite titanates $ATiO_3$ ($A=Ca, Sr, Ba, Pb, Eu$) where the A sites are occupied by +2 ions. In spite of the largely ionic character of these ions, the properties of these compounds differ substantially. They range from order/disorder like, to displacive ferroelectric, quantum paraelectric, and antiferromagnetic. All compounds crystallize in the cubic structure at high temperature and undergo structural phase transitions to tetragonal symmetry, partly followed by further transitions to lower symmetries. Since the TiO_6 moiety is the essential electronic and structural unit, the question arises, what makes the significant difference between them. It is shown that the lattice dynamics of these compounds are very different, and that mode-mode coupling effects give rise to many distinct properties. In addition, the oxygen ion nonlinear polarizability plays a key role since it dominates the anharmonicity of these perovskites and determines the structural instability.

*Corresponding author: a.bussmann-holder@fkf.mpg.de

Half-metallic states in a doped density-wave insulator

A.V. Rozhkov^{1,2}, A.L. Rakhmanov^{1,2,3}, A.O. Sboychakov¹, K.I. Kugel^{*1,4},
and F. Nori⁵

¹*Institute for Theoretical and Applied Electrodynamics, Russian Acad. Sci., Moscow, 125412 Russia*

²*Moscow Institute for Physics and Technology (State University), Moscow region, 141700 Russia*

³*Dukhov Research Institute of Automatics, Moscow, 127055 Russia*

⁴*National Research University Higher School of Economics, Moscow, 109028 Russia*

⁵*Center for Emergent Matter Science, RIKEN, Wako-shi, Saitama, 351-0198, Japan*

Half-metals are rather unusual and promising materials. The Fermi surface of a half-metal is completely spin-polarized. Namely, electronic states with only one spin projection value reach the Fermi energy. States with the other spin projection are pushed away from the Fermi level. This makes half-metals useful for spintronics. Typically, half-metallicity arises in strongly correlated electron systems, or when localized magnetic moments are present. Here, we demonstrate that doping a density-wave insulator even in the weak-coupling limit may stabilize new types of half-metallic states, such as spin-valley half-metal and charge-density wave (CDW) half-metal [1].

In our analysis is based on a simple model Hamiltonian describing charge carriers belonging to two bands: electron band a and hole band b . Both bands have the parabolic dispersion law and spherical Fermi surface pockets (or valleys). When the Fermi surface valleys nest well (that is, the Fermi momentum of electrons a equals to the Fermi momentum of holes b), the electron-electron repulsion generates spin- or charge-density wave state. This ordered mean-field ground state is unique up to symmetry transformations, for example, spin rotations.

If charge is added or removed from such a system, the situation becomes less clear-cut: it is believed that at finite doping level, several states with close energies compete against each other to become a true ground state. Several possibilities are discussed in the theoretical literature: incommensurate density wave, electronic phase separation, stripes, etc. We demonstrate that yet another type of many-body state is available. In the doped system, the two-valley Fermi surface emerges. One valley is electron-like. It is composed mostly of states of band a with spin σ . Another valley is hole-like, composed predominantly of states of band b with spin σ' . These Fermi surface valleys have half-metallic character: the states in band a with spin $-\sigma$, as well as states in band b with spin $-\sigma'$, do not reach the Fermi level and have no Fermi surface.

Depending on the parameters, the spin polarizations of the electron-like valley and hole-like valley may be parallel ($\sigma = \sigma'$) or antiparallel ($\sigma = -\sigma'$). The former case is similar to the usual half-metal: quasiparticles at the Fermi surface are completely spin-polarized. In addition, the system exhibits a finite CDW order parameter. For this reason, we refer to such a state as the CDW half-metal. When $\sigma = -\sigma'$, the total spin polarization averages to zero. It is proven, however, that in this situation, the so-called spin-valley polarization is nonzero. Thus, the state is called the spin-valley half-metal. The specific features of these half-metallic states are discussed.

- [1] A.V. Rozhkov, A.L. Rakhmanov, A.O. Sboychakov, K.I. Kugel, and F. Nori, "Spin-valley half-metal as a prospective material for spin valleytronics", *Phys. Rev. Lett.* **119**, 107601 (2017).

*Corresponding author: klimkugel@gmail.com

Spin-charge conversion at oxide interfaces

G. Seibold*¹, S. Caprara², M. Grilli², and R. Raimondi³

¹*Institut für Physik, BTU, Cottbus-Senftenberg, P.O. Box 101344, 03013 Cottbus, Germany*

²*Dipartimento di Fisica Università di Roma 'La Sapienza', Piazzale Aldo Moro 5, I-00185 Roma, Italy*

³*Dipartimento di Matematica e Fisica, Università Roma Tre,
Via della Vasca Navale 84, 00146 Rome, Italy*

The manipulation of spin degrees of freedom in order to generate a charge current and the inverse process are at the heart of spintronics devices. A prominent example is the spin-galvanic effect (SGE) where a charge current is converted into a non-equilibrium spin polarization. The SGE occurs in systems with strong spin-orbit coupling, in particular two-dimensional electron gases which lack inversion symmetry perpendicular to the gas plane and which are usually described with the Rashba hamiltonian. The situation is more complex in LaAlO₃/SrTiO₃ interfaces where the interplay between inversion asymmetry and atomic spin orbit coupling is at the heart of strong Rashba interactions. Recently, two experiments [1,2] have demonstrated a strong SGE at such interfaces by generating a strong non-equilibrium spin-polarization at the interface and detecting the resulting charge current. The reported spin-to-charge efficiency is more than order of magnitude larger than in conventional metallic layers which suggests the LAO/STO interface as a promising system for spintronic devices.

Here, we analyze the SGE for oxide interfaces within a tight-binding three-band model for the Ti t_{2g} orbitals, where we take into account atomic spin-orbit coupling and the lifting of inversion symmetry at the interface. As a result, the model displays an interesting variety of effective spin-orbit couplings in the individual bands that contribute differently to the spin-to-charge interconversion [3].

As a first step we derive an effective continuum Hamiltonian describing three spin-orbit split bands close to the Gamma point. Within such an effective model, we study the SGE by using the standard Green-function diagrammatic impurity technique for disordered electron systems. Our analytical approach is supplemented by a numerical evaluation of the Kubo formula for the spin polarization-charge current response. The numerical treatment evidences the importance of interband scattering processes, not taken into account in the effective model. Within the numerical treatment we also investigate the influence of disorder and temperature, which turns out to be crucial in providing an appropriate description of the experimental data.

[1] Lesne et al., Nature Materials **15**, 1261 (2016).

[2] Q. Song et al., Nature Communications, 10.1038 (2016).

[3] G. Seibold et al., Phys. Rev. Lett. **119**, 256801 (2017).

*Corresponding author: seibold@b-tu.de

London penetration depth in the ensemble of spin-polarons of cuprate superconductors

D.M. Dzebisashvili*^{1,2} and K.K. Komarov¹

¹Kirensky Institute of Physics, Federal Research Center KSC SB RAS, 660036 Krasnoyarsk, Russia

²Reshetnev Siberian State University of Science and Technology, 660037 Krasnoyarsk, Russia

The explanation for unusual properties of cuprate high-temperature superconductors is based on the strong electron correlations, which lead, in particular, to a significant coupling between charge and spin degrees of freedom. A spin-polaron approach, developed in [1], allows correctly take into account the specific features of cuprate HTSCs. Within this approach the spectral properties of cuprates at low temperatures were studied [1,2], and the evolution with doping of the Fermi surface in the form of a "hole pocket" in the vicinity of the point $(\pi/2, \pi/2)$ of the Brillouin zone was described [3].

An important advance in the spin polaron concept occurred when a theory of the Cooper instability in the ensemble of spin polarons with d-wave order parameter was developed [4]. In particular there was established a very important fact that the Coulomb interaction between holes on the nearest oxygen ions does not affect the d-wave superconductivity in cuprates, since the Fourier transform of this interaction falls out of the equation for the corresponding order parameter [5]. Also, it was recently shown [6] that s-wave superconductivity does not arise within the spin-polaron approach since the equation for the s-wave order parameter does not have nontrivial solutions. Together the obtained results allowed to solve: 1) the problem of s-phase domination in the theory of cuprates that contradicts experiment; 2) the long standing problem of suppressing the d-wave solutions by the intersite Coulomb interactions.

In the present work, by calculating the London penetration depth λ_L , it is shown that the spin-polaron approach allows one to describe successfully also the electrodynamic properties of cuprate HTSCs. To study the concentration and temperature dependence of λ_L , a novel method was proposed to derive the superconducting current in the ensemble of spin-polaron quasiparticles due to uniform field of the vector potential $A_{q=0}$. Unlike the conventional methods, this method: 1) does not imply the analytical expression for quasiparticle spectrum to be known; 2) is applicable to multi-band systems; 3) is not limited to small values of $A_{q=0}$. The calculated concentration and temperature dependences of λ_L are compared to the available experimental data on cuprates.

The work was supported by the Russian Foundation for Basic Research (grant no. 18-02-00837) and the Program of Presidium of the Russian Academy of Sciences No.12 "Fundamental Problems of High-temperature Superconductivity". The work of K.K.K. was supported by the Council for Grants of the President of the Russian Federation (MK-1398.2017.2).

- [1] A.F. Barabanov, V.M. Berezovskii, E. Zhasinas, L.A. Maksimov, "On the origin of the saddle in the spectrum of holes in a CuO₂ plane" *JETP*, **83** (4), 819-828 (1996).
- [2] A.F. Barabanov, R.O. Kuzian, L.A. Maksimov, "Spectral function of small spin polaron in two-dimensional spherically symmetric antiferromagnetic state" *Phys. Rev. B*, **55** (7), 4015-4018 (1997).
- [3] D.M. Dzebisashvili, V.V. Val'kov, A.F. Barabanov, "Fermi surface evolution in the ensemble of spin-polaron quasiparticles in La_{2-x}Sr_xCuO₄." *JETP Letters*, **98** (9), 596-601 (2013).
- [4] V.V. Val'kov, D.M. Dzebisashvili, A.F. Barabanov, "d-wave pairing in an ensemble of spin polaron quasiparticles in the spin-fermion model of the electronic structure of the CuO₂-plane" *Phys. Lett. A*, **379** (5), 421-426 (2015).
- [5] V.V. Val'kov, D.M. Dzebisashvili, M.M. Korovushkin, A.F. Barabanov, "Stability of the superconducting d_{x²-y²}-phase in High-Tc superconductors with respect to the intersite Coulomb repulsion of holes at oxygen" *JETP Letters*, **103** (6), 433-437 (2016).
- [6] V.V. Val'kov, D.M. Dzebisashvili, M.M. Korovushkin, A.F. Barabanov, "Coulomb repulsion of holes and competition between d_{x²-y²}- and s-wave parings in cuprate superconductors" *JETP*, **125** (5), 810-821 (2017).

*Corresponding author: ddm@iph.krasn.ru

Underdoped/Overdoped symmetry of cuprate superconductors

Jürgen Röhler*¹

¹Universität zu Köln, Fachgruppe Physik, 50937 Köln, Germany

The superfluid density ρ_s in disorder free and clean overdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ ($0.25 > x > 0.19$) was recently established from measurements of the penetration depth (λ) to scale with T_c [1]. Linear $\rho_s(T)$ at all dopings rules out disorder-based explanations. The complex conductivity in the THz range exhibits a broad Drude-like peak down to $T = 0$ [2] that indicates a significant fraction of the normal carriers to remain in fact uncondensed. These results challenge the widely held expectation that the physics of overdoped cuprates may be understood using the standard 'dirty' d -wave BCS formalism.

We address the underdoped/overdoped symmetry of the universal relationship between T_c and ρ_s in cuprate superconductors investigating an Ansatz related to the RVB theory wherein mobile holes created under the constraint of on-site non double occupancy are excluded from nearest neighbor hole sites. Through the underdoped regime up to $p_{\text{opt}} < 1/6$ the constraining organization of hole pairs increases the superfluid stiffness. At densest (tweedy) packing of the bond centered hole pairs a remarkable kink is exhibited, likely related to the ubiquitous maximum of the condensation energy around $p^* \sim 0.19$. Beyond p^* the superfluid stiffness decreases until it vanishes at $p_{\text{opt}} = 1/4$. Overdoped holes exceed densest packing [3] hence must be accommodated in site centered configurations that will unlock hole pairs from the local inversion symmetry of the spin singlets in the RVB liquid.

- [1] I. Bozovic, X. He, J. Wu, A. T. Bollinger, *Nature* **536**, 309 (2016).
- [2] F. Mahmmod, X. He, I. Bozovic, N. P. Armitage., arXiv:1802.02101 (2018).
- [3] J. Röhler, *Int. J. Phys* **19**, 255 (2005).

*Corresponding author: juergen.roehler@uni-koeln.de

1D-, 2D-, and 3D-Topological Laser Solitons

N.N. Rosanov*^{1,2}, S.V. Fedorov^{1,2}, and N.A. Veretenov^{1,2}

¹*Vavilov State Optical Institute, Birzhevaya liniya 12, St. Petersburg, 199034 Russia*

²*St. Petersburg State University of Information Technologies, Mechanics, and Optics, St. Petersburg, 197101 Russia*

*Corresponding author: nnrosanov@mail.ru

Investigation of subsonic crowdion induced mass transfer in metals

Igor A. Shepelev*¹, Elena A. Korznikova², Alexander P. Chetverikov¹, and Sergey V. Dmitriev^{2,3}

¹*Saratov Chernyshevsky State University, Astrakhanskaya Ulitsa, 83, 410012, Saratov, Russia*

²*Institute for Metals Superplasticity Problems of RAS, Khalturin St. 39, 450001 Ufa, Russia*

³*National Research Tomsk State University, Lenin Avenue 36, 634050 Tomsk, Russia*

Design of new approaches for mass transfer enhancement in crystals in non-equilibrium conditions requires a deep understanding of the role and mechanisms of lattice defects in this process. It is well known that point defects play a very important role in processes of energy dissipation in crystals subjected to plastic deformation, irradiation, plasma treatment, etc. Their basic properties and role in the mass transfer can be studied in frame of simplified crystal models.

We have performed a molecular dynamics study of crowdion type defect formation induced by initial kick of several small atom group configurations along the closely packed atomic row in Morse crystal without on site potential. It was shown that applying initial displacement to a group of atoms in all cases results in formation of one or several vacancies and interstitials or crowdion type defects depending on the initial conditions. The investigation revealed that in all analyzed cases one can observe moving breathing crowdions having own localized vibrational mode with the frequency above the phonon band of the crystal.

Detailed study of the scenario of time evolution of the energy distribution in the lattice revealed that in case of one atom initiation the resulting crowdion is only stable when moving and the deceleration results in its transformation to an interstitial atom. Increase of the number to $N = 2$ of atoms in the group subjected to kick leads to formation of two subsonic crowdions moving in the direction of the initial kick. Further increase of N up to 3 atoms in the group shows the similar behavior of lattice dynamics including formation of two subsonic crowdions and a double - vacancy. One should also mention that after definite time of simulation the progressive movement of crowdions is slackened and followed by the movement in the opposite direction. This fact can be explained by the stress field of the bivacancy created by the initial kink of three atoms and creating the long range elastic stresses attracting the opposite sign defects.

The efficiency of mass transfer by crowdions for different initial conditions and reasons for variety of behavior scenarios will be discussed.

*Corresponding author: igor_sar@li.ru

Monte Carlo Simulations of Sn induced defects on the Ge(001) surface reconstruction

Katharina Noatschk*¹, Wolfgang M. Klesse², Jaroslaw Dabrowski², Emily Hofmann², Thomas Schroeder^{1,2}, and Götz Seibold¹

¹Brandenburg Technical University Cottbus-Senftenberg, 03046 Cottbus, Germany

²IHP, 15236 Frankfurt(Oder), Germany

A direct band gap is obtained by the formation of Ge-Sn alloys with a Sn content of at least 8%, presenting a direct bandgap group IV semiconductor potentially compatible with state-of-the-art CMOS fabrication [1]. From an experimental point of view the growth of high quality GeSn films provides many challenges, because in thermodynamic equilibrium (below 773.15 K) the solubility of Sn in Ge is limited to 1%. For example, to suppress Sn segregation or severe surface roughing during growth non-thermal equilibrium processes are required, by utilizing low growth temperatures, high growth rates or even strain engineering of thin films [2].

In this context, theoretical approaches, in particular kinetic Monte Carlo Simulations, may provide crucial control parameters and assist in the exploration of alternative growth strategies. However, before the actual GeSn growth can be investigated by kinetic Monte Carlo Simulations, first an experimentally realistic Ge(001) surface must be accurately modeled, including the possible surface reconstructions (i.e. $c(4 \times 2)$, $p(2 \times 2)$, $p(4 \times 1)$ and $p(2 \times 1)$), formed by the buckled dimerization of surface atoms [3]. Hereby motivated, we present Monte Carlo Simulations on the stability of the different reconstructions as well as the influence of Sn-defects on the Ge(001) surface reconstruction by using varying Sn concentrations (i.e. 0.5%, 5% and 20%). For the stability analysis of the defect-free Ge(001) surface we assume that in equilibrium the tilting angle of each dimer has two possible states only. Therefore, the frustrated Ising Model has proven an effective model [4], which can be solved by using Monte Carlo Simulations. In agreement with experimental observations, our calculations confirm the $c(4 \times 2)$ reconstruction as the most stable one with a phase transition temperature of 310 K (see figure 1(a)). Furthermore, our Monte Carlo Simulations reveal the formation on distinct sign domains of the buckled dimer orientation on the surface, as show in figure 1(b). Finally, we show that one sign domain will be preferred by Sn-impurities.

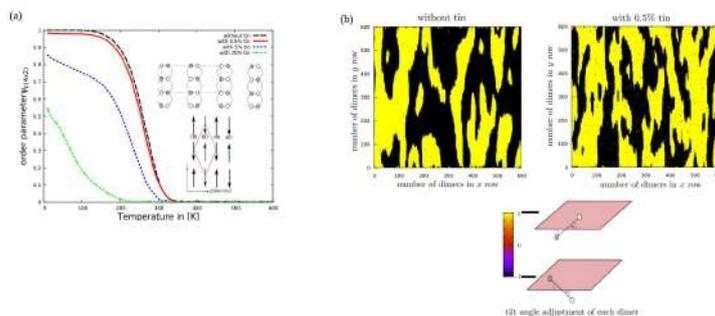


Figure 1: (a) shows that the $c(4 \times 2)$ reconstruction is stable at 310 K and (b) shows the surface structure of the $c(4 \times 2)$ reconstruction at 100 K with sign domains without and with tin.

- [1] R.A.S.a.L. Friedman, *Superlattices Microstruct.*, p. 189, 1993
- [2] Sigeaki Zaima et al., *Sci. Technol. Adv. Mater.* 16, 043502 (22pp), 2015
- [3] Guang-Hong Lu et al., *Surface Science* 588, 61-70, 2005
- [4] Y. Yoshimoto, Y. Nakamura, H. Kawai, M. Tsukada, M. Nakayama, *Phy. Rev. B* Vol. 61, Num. 2000-I

*Corresponding author: Katharina.Noatschk@b-tu.de

Canted Screw-Type Motion and Dynamics of the Electronic Ground State in Low-Dimensional Fe(II) Compounds

A. Möller*¹, A. Reuß¹, V. Ksenofontov¹, D. Wulferding², and P. Lemmens²

¹*Institute for Inorganic and Analytical Chemistry, JGU Mainz,
Duesbergweg 10-14, 55128 Mainz, Germany*

²*Institute for Condensed Matter Physics, TU Braunschweig,
Mendelssohnstr. 3, 38106 Braunschweig, Germany*

We will present our recent results on selected low-dimensional Fe(II) compounds in terms of cooperative effects originating from electron-phonon coupling. The evaluation of the apparent dynamics is based on a combination of temperature dependent x-ray diffraction, Mössbauer and Raman spectroscopic measurements. Specifically, we have identified certain principal lattice modes which lead to an effective canted screw-type motion of the vanadate groups in these compounds. Ultimately, the collective component of the lattice dynamics with the electronic ground state of Fe(II) drives a structural transition at elevated temperatures on the triangular lattice. Furthermore, we will comment on the dynamics in the magnetically correlated temperature regime. Additional aspects of structure-property relationships in this family of compounds ($AB_2M[VO_4]_2$ with A = alkaline or alkaline-earth metal, B = sodium or silver, and M = 3d-transition metal) can be found in references [1-3].

- [1] J. Tapp, C. R. dela Cruz, M. Bratsch, N. E. Amuneke, L. Postulka, B. Wolf, M. Lang, H. O. Jeschke, R. Valentí, P. Lemmens, A. Möller, "From magnetic order to spin liquid ground states on the $S = 3/2$ triangular lattice", *Phys. Rev. B* **96**, 064404 (2017).
- [2] N.E. Amuneke, J. Tapp, C. dela Cruz, A. Möller, "Experimental Realization of a Unique Class of Compounds: XY-Antiferromagnetic Triangular Lattices, $KAg_2Fe[VO_4]_2$ and $RbAg_2Fe[VO_4]_2$, with Ferroelectric Ground States", *Chem. Mater.* **26**, 5930 (2014).
- [3] M. Bratsch, A.P. Litvinchuk, J. Tapp, A. Möller, "Synthesis, Thermodynamic and Spectroscopic Properties of Honeycomb-Type Lattices: $AAg_2(M'_{1/3}M_{2/3})[VO_4]_2$ ", *Inorg. Chem.* **53**, 4994 (2014).

*Corresponding author: angela.moeller@uni-mainz.de

Isotropic helical states in frustrated magnetism: continuous transitions on the J_1 - J_2 - J_3 globe

V.E. Valiulin^{1,2,3}, A.V. Mikheyenkov^{*1,2,3}, N. M. Chtchelkatchev^{1,2,4,5}, and
A.F. Barabanov¹

¹*Institute for High Pressure Physics, Russian Academy of Sciences, Moscow (Troitsk) 108840, Russia*

²*Moscow Institute of Physics and Technology, Moscow 141700, Russia*

³*National Research Centre "Kurchatov Institute", Moscow 123182, Russia*

⁴*L.D. Landau Institute for Theoretical Physics, Russian Academy of Sciences, Moscow 119334, Russia*

⁵*Institute of Metallurgy, Ural Branch, Russian Academy of Sciences, Ekaterinburg 620016, Russia*

Frustrated magnetic compounds, in particular, low-dimensional, are topical research due to persistent uncover of novel nontrivial quantum states and potential applications. The problem of this field is that many important results are scattered over the localized islands of parameters, while nebular areas in between still contain hidden new physics. We have found new local order in spin liquids: antiferromagnetic isotropical helices. On the structure factor we see gyrate concentric dispersionless structures, while on any radial direction the structure factor has "roton" minima. That implies nontrivial magnetic excitations and consequences in magnetic susceptibility and thermodynamics. On the J_1 - J_2 - J_3 exchanges globe we discover a continuous pass from antiferromagnetic-like local order to ferromagnetic-like; we find stripe-like order in the middle of this pass. In fact, our "quasielastic" approach allows investigation of the whole J_1 - J_2 - J_3 globe [1].

As an example, we have calculated [2] in the frames of J_1 - J_2 - J_3 model the heat capacity and magnetic susceptibility of the quasi-two-dimensional square-lattice compound $(\text{CuBr})\text{Sr}_2\text{Nb}_3\text{O}_{10}$, where neutron experiment indicates helical spin order while common explanation by Dzyaloshinskii-Moriya interaction is unacceptable [3-5]. The results show good agreement with the experiment.

- [1] A.V. Mikheenko, V.E. Valiulin, A.V. Shvartsberg, A.F. Barabanov, "Helical Quantum States in a Strongly Frustrated Two-Dimensional Magnet", JETP, **126** (3), 405-417 (2018).
- [2] A.V. Mikheenko, V.E. Valiulin, A.V. Shvartsberg, A.F. Barabanov, "Magnetic spiral order in the square-lattice spin system $(\text{CuBr})\text{Sr}_2\text{Nb}_3\text{O}_{10}$ ", submitted to JMMM.
- [3] S.M. Yusuf, A.K. Bera, C. Ritter *et al.*, "Magnetic correlation in the square-lattice spin system $(\text{CuBr})\text{Sr}_2\text{Nb}_3\text{O}_{10}$ ": A neutron diffraction study, Phys. Rev. B **84** (6) (064407 (2011)).
- [4] Y. Tsujimoto, Y. Baba, N. Oba, H. Kageyama *et al.*, "1/3 Magnetization Plateau in Spin-1/2 Square Lattice Antiferromagnet $(\text{CuBr})\text{Sr}_2\text{Nb}_3\text{O}_{10}$ ", J. Phys. Soc. Jpn. **76** (6) (2007) 063711 (2007).
- [5] C. Ritter, S.M. Yusuf, A.K. Bera *et al.*, "Field-induced evolution of magnetic ordering in the quantum spin system $(\text{CuBr})\text{Sr}_2\text{Nb}_3\text{O}_{10}$ with a 1/3 magnetization plateau", Phys. Rev. B **88** (10) 104401 (2013).

*Corresponding author: mikheen@bk.ru

The inversion probability of a large spin as an asymptotic expansion in series of Bessel functions

Ekaterina A. Karatsuba*¹ and Paolo Moretti²

¹Federal Research Center "Computer Science and Control" of RAS,
ul. Vavilova 40, 119991 Moscow, Russia

²Istituto dei Sistemi Complessi del C.N.R. Sezione di Firenze,
via Madonna del Piano 10, 50019 Sesto Fiorentino, Italy

Spin dynamics plays a very important role in the study of molecular magnetic clusters. In particular, if Mössbauer spectroscopy is used, the inversion time of the spin is one of the most important parameters in the structure of experimental spectra [1].

To find the probability amplitude of the spin inversion in [2] was constructed a new model in which a set of equations was solved by Laplace transform. The coefficient $|b_n(t)|^2$ which gives the probability of finding the system in n -th spin state, was found in [2] in the form of the following involute trigonometric sum

$$b_n(t) = -2 \frac{(-1)^n}{N+1} \sum_{s=1}^N \sin \frac{s\pi}{N+1} \sin \frac{ns\pi}{N+1} \exp \left[2i \frac{k}{\hbar} t \cos \frac{s\pi}{N+1} \right],$$

and an approximation for $b_n(t)$ was obtained with such restrictions that $n \ll N$, $\alpha t \ll N$ (α is a parameter). Here N is the total number of spin states, $1 \leq n \leq N$.

The presented talk is about study of the behavior of the function $b_N(t)$ for $N \geq 2$. A new formula for the probability amplitude $b_N(t)$ for any t and $N \geq 2$ is derived. This exact expression in terms of Bessel's functions with large indexes provides an effective computation of $b_N(t)$ with increasing accuracy. New formula for the inversion time is obtained. The results were published in [3]. Some following experimental studies on molecular magnets [4,5] assume that the use of this theory is suitable in the case of magnetic molecular clusters, for the problem concerning the nature of the basic mechanism of the spin dynamics. This is an important issue, since spin fluctuations affect magnetization.

- [1] Blume M., Tjon J.A. Mössbauer Spectra in a Fluctuating Environment. *Phys. Rev.* **165**, 2, 446 (1968).
- [2] Moretti P., Lantieri M. and Cianchi L., Quantum study of the spin inversion. *J. Math. Phys.*, **45**, 1, 107 (2004).
- [3] Karatsuba E.A., Moretti P., Inversion time of large spins. *J. Math. Phys.*, 46, 4, 042101 (2005).
- [4] Cianchi L., Del Giallo F., Lantieri M., Moretti P., Spina G., Study of the $[\text{Fe}(\text{OMe})(\text{dpm})_2]_2$ dimer in the presence of a magnetic field by using Mössbauer spectroscopy. *Hyp. Int.*, **168**, 1115 (2006).
- [5] Cianchi L., Del Giallo F., Moretti P., Spina G., Mancini M., Caneschi A., Lantieri M., Magnetic anisotropy and spin fluctuations in the paramagnetic dimer $[\text{Fe}(\text{OMe})(\text{dpm})_2]_2$: Mössbauer spectroscopy and *ab initio* calculations. *J. Magn. Magn. Mater.*, **320**, 898 (2008).

*Corresponding author: ekar@ccas.ru, karacuba@mi.ras.ru

Nonlinear excitations in arrays of magnetic dots

Y. Zolotaryuk*¹

¹*Bogolyubov Institute for Theoretical Physics, National Academy of Sciences of Ukraine,
Kyiv 03680, Ukraine*

The dynamics of ferromagnetic arrays of magnetic particles (dots) with the easy-plane anisotropy is investigated. The particles interact with each other via the magnetic dipole interaction and the whole system is governed by the system of coupled Landau-Lifshitz equations. We demonstrate existence of spatially localized and time-periodic solutions known as discrete breathers (or intrinsic localized modes) that have no analogue in the continuum limit and are reminiscent to the discrete breathers in Heisenberg ferromagnets, studied previously [1]. These solutions have the following structure: (i) the core, where the magnetization vectors precess around the hard axis, and, (ii) the tails, where the magnetization vectors oscillate around the equilibrium position. The allowed breather frequencies spectrum bounded from above by the value of the hard axis component of the magnetic moment and from below it is bounded by the maximal magnon frequency. The existence diagram on the parameter plane “frequency-discreteness constant” has been constructed.

- [1] Y. Zolotaryuk, S. Flach and V. Fleurov, *Phys. Rev. B* **63**, 214422(12) (2001);
J.M. Khalack, Y. Zolotaryuk and P.L. Christiansen, *CHAOS* **13**, 683-692 (2003).
- [2] R. L. Pylypchuk and Y. Zolotaryuk, *Low Temp. Phys.* **41**, 733-738 (2015).

*Corresponding author: yzolo@bitp.kiev.ua

Spin liquid and dimerization in the Kitaev hyperhoneycomb magnet β -Li₂IrO₃

A.A. Tsirlin*¹

¹*Experimental Physics VI, Center of Electronic Correlations and Magnetism, University of Augsburg*

Kitaev spin liquid remains an intriguing and elusive state of matter that has never been realized experimentally. Honeycomb and honeycomb-related iridates and ruthenates, the best real-world prototypes of Kitaev magnets, all show long-range magnetic order in zero field. Nevertheless, it is conjectured that pressure may tune these materials away from the magnetically long-range-ordered state and, potentially, toward the spin liquid.

Here, we test this conjecture using x-ray diffraction, thermodynamic measurements, and muon spin relaxation (μ SR) on hyperhoneycomb β -Li₂IrO₃ under pressure [1]. No structural changes are seen up to 3.5 GPa, whereas magnetic behavior changes drastically. The Néel temperature increases up to about 1.4 GPa, where magnetic order disappears abruptly. The field-induced transition between the incommensurate and zigzag-correlated states shifts toward lower fields, thus reflecting an increasing instability of the incommensurate order. Indeed, μ SR suggests magnetic order collapse around 1.4 GPa, and reveals the coexistence of static (frozen) and dynamic spins above this pressure. We interpret this novel pressure-induced state as a partially frozen spin liquid. Interestingly, the freezing occurs in the absence of any visible structural defects. This fact may indicate classical nature of the pressure-induced spin liquid. The evolution of the exchange parameters probed by quantum-chemical (cluster) and density-functional (periodic) calculations shows the increase in the off-diagonal Γ exchange term that may become the leading term under pressure and drives the system toward the classical spin-liquid state [2].

A structural phase transition takes place around 3.7 GPa. Crystal symmetry changes from orthorhombic to monoclinic, and some of the Ir-Ir distances shorten to 2.6 Å, which is less than the interatomic distance in the Ir metal and indicates the formation of metal-metal bonds. This pressure-induced dimerization is generic for honeycomb iridates [3]. Our density-functional calculations reveal the crucial role of both Coulomb repulsion and Hund's coupling in stabilizing the dimerized phase.

[1] M. Majumder *et al.* arXiv:1802.06819

[2] I. Rousochatzakis and N. Perkins, Phys. Rev. Lett. 118, 147204 (2017).

[3] V. Hermann *et al.* Phys. Rev. B 97, 020104(R) (2018).

*Corresponding author: altsirlin@gmail.com

Spin-orbital model of stoichiometric LaMnO_3 with tetragonal distortions

Andrzej M. Oleś^{*1,2} and Mateusz Snamina³

¹Marian Smoluchowski Institute of Physics, Faculty of Physics, Astronomy, and Applied Comp. Science, Jagiellonian University, Prof. S. Łojasiewicza 11, PL-30348 Kraków, Poland

²Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

³Kazimierz Gumiński Department of Theoretical Chemistry, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, PL-30387 Kraków, Poland

In LaMnO_3 strong intraorbital Coulomb repulsion U localizes electrons and the effective interactions between Mn^{3+} ions in $t_{2g}^3 e_g^1$ configuration take the form of spin-orbital superexchange [1]. *A priori* spin-orbital degrees of freedom are entangled [2], yet the separation of these degrees of freedom is frequently done and the results of such calculations agree well with experiment. Here we address this situation and establish by cluster mean field analysis that the spin-orbital entanglement is rather weak for both on-site and on-bond quantities [3]. We have used several cluster mean field calculation schemes and find coexisting *A*-type antiferromagnetic (*A*-AF) and *C*-type alternating orbital (*C*-AO) order at low temperature. The Jahn-Teller (JT) coupling between strongly correlated e_g orbitals influences the orbital transition at $T_{OO} \sim 780$ K and is estimated as intermediate. We have verified that the magnetic transition temperature is influenced by entangled spin-orbital operators as well as by entangled orbital operators on the bonds but the errors introduced by decoupling such operators partly compensate each other. Altogether, these results justify why the commonly used disentangled spin-orbital model is so successful in describing the magnetic properties and the temperature dependence of the optical spectral weights for LaMnO_3 . The most important prediction at finite temperature is that the spectral weights become isotropic above the orbital transition temperature $T_{OO} \sim 780$ K.

The model for LaMnO_3 [1] explains the *A*-AF/*C*-AO order by a combination of superexchange and JT interactions in a cubic (perovskite) symmetry, whereas real crystal structure is strongly deformed. We identify three effects arising from tetragonal deformation:

- (i) the crystal-field splitting of e_g orbitals $\sim E_z$,
- (ii) the directional renormalization of d - p hybridization $\sim t_{pd}$, and
- (iii) the directional renormalization of charge excitation energies,

and evaluate their magnitude [4]. It is found that the major effects of deformation are enhanced amplitude of $x^2 - y^2$ orbitals induced in the *C*-AO order by $E_z=300$ meV and anisotropic $t_{pd}=2.0$ (2.35) eV within the *ab* planes (along the *c* cubic axis), in very good agreement with the Harrison's law. We show that the tetragonal model analyzed within mean field approximation provides a surprisingly consistent picture of the ground state of LaMnO_3 . Excellent agreement with the experimental data is obtained for: (i) e_g orbital mixing angle, (ii) spin exchange constants, and (iii) the temperatures of spin T_N and orbital T_{OO} phase transition.

We acknowledge support by Narodowe Centrum Nauki (NCN) under Project No. 2016/23/B/ST3/00839.

- [1] L. F. Feiner and A. M. Oleś, "Electronic origin of magnetic and orbital ordering in insulating LaMnO_3 ", *Phys. Rev. B* **59**, 3295 (1999).
- [2] A. M. Oleś, "Fingerprints of spin-orbital entanglement in transition metal oxides", *J. Phys.: Condensed Matter* **24**, 313201 (2012).
- [3] M. Snamina and A. M. Oleś, "Spin-orbital order in the undoped manganite LaMnO_3 at finite temperature", *Phys. Rev. B* **94**, 214426 (2016).
- [4] M. Snamina and A. M. Oleś, "Spin-orbital model of stoichiometric LaMnO_3 with tetragonal distortions", *Phys. Rev. B* **97**, 104417 (2018).

*Corresponding author: a.m.oles@fkf.mpg.de

Phonons probe topological degrees of freedom in Dirac and Weyl semimetals

P. Lemmens^{*1,2}, A. Sharafeev¹, V. Gnezdilov^{1,3}, R. Sankar^{4,5}, and F.C. Chou⁴

¹*Inst. for Condensed Matter Physics, TU Braunschweig, D-38106 Braunschweig, Germany*

²*Laboratory for Emerging Nanometrology, TU Braunschweig, D-38106 Braunschweig, Germany*

³*B.I. Verkin Inst. for Low Temp. Phys. and Engineering, NASU, Kharkov 61103, Ukraine*

⁴*Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan*

⁵*Institute of Physics, Academia Sinica, Nankang, Taipei 11529, R.O.C. Taiwan*

Weyl and Dirac semimetals are three dimensional phases of matter with gapless electronic excitations that are protected by topology and symmetry [1]. Due to the analogy to graphene, unconventional transport properties, and a relation to particle physics models of relativistic chiral fermions they generated considerable interest in the solid state physics community.

Despite these electronic properties there are also relations to bosonic degrees of freedom, e.g. there exist mechanical systems that mimic protected excitations. Recently, it has also been shown that inter- and intraband excitations within topological electronic states of Weyl and Dirac semimetals couple to phonons leading to self-energy contributions as function of the momentum of the phonon [2,3]. In this sense phonons can characterize topological degrees of freedom of the electronic system.

In our Raman scattering study on several Weyl and Dirac semimetals we will show that such effects can be observed experimentally as anharmonic variations of the phonon linewidth and frequency as function of temperature. A model system with this respect is the three-dimensional Dirac semimetal Cd_3As_2 [4]. However, we will also discuss other materials.

We thank David Schmeltzer and Ion Garate for important discussions. We would like to acknowledge the support of the International Graduate School of Metrology (B-IGSM) and the Graduate School "Contacts in Nanosystems". Financial support by GIF and DFG-RTG 1952 Nanomet, and DFG-LE967/16-1 is appreciated. FCC acknowledges support from the Ministry of Science and Technology in Taiwan under grant No. MOST-104-2119-M-002 -028-MY2.

[1] N.P. Armitage, E.J. Mele, Ashvin Vishwanath, *Rev. Mod. Phys.* **90**, 15001 (2018).

[2] I. Garate, *Phys. Rev. Lett.* **110**, 46402 (2013).

[3] K. Saha, K. Légaré, and I. Garate, *Phys. Rev. Lett.* **115**, 176405 (2015).

[4] A. Sharafeev, V. Gnezdilov, R. Sankar, F.C. Chou, and P. Lemmens, *Phys. Rev. B* **95**, 235148 (2017).

*Corresponding author: p.lemmens@tu-bs.de

NMR investigation of the frustrated spin chain compound β -TeVO₄

R. Stern^{*1}, I. Heinmaa¹, F. Weickert², M. Jaime², H. Berger³, O. Janson^{1,4},
and A.A. Tsirlin^{1,5}

¹National Institute of Chemical Physics and Biophysics, 12618 Tallinn, Estonia

²MPA-CMMS, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

³Ecole Polytechnique Fédérale de Lausanne, Lausanne CH-1015, Switzerland

⁴Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

⁵Experimental Physics VI, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

In strongly correlated electron systems, the presence of motifs of periodic modulations has typically been associated with competition between short- and long-range interactions. Here we show that spin-stripe textures develop also in antiferromagnets, in our case in β -TeVO₄, a nearly ymodel with FM J_1 and antiferromagnetic (AFM) J_2). A narrow spin-stripe phase develops at elevated magnetic fields due to weak frustrated short-range inter-chain exchange interactions, possibly assisted by the symmetry-allowed electric polarization. This concept provides an alternative route for the stripe formation in strongly correlated electron systems and may help understanding of other widespread, yet still elusive, stripe-related phenomena.

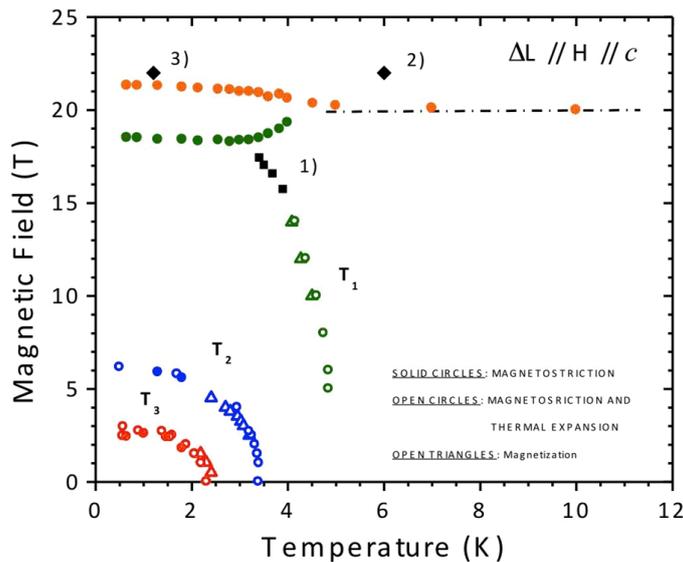


Figure 1: Field-Temperature phase diagram for β -TeVO₄ when the magnetic field is applied along crystallographic $\langle 001 \rangle$. Black dots (1) are evaluated from the divergence of ¹²⁵Te spin-spin relaxation T_2 rate.

The phase diagram displayed in Fig. 1 reveals previously unknown anisotropy, and the possibility of a tri-critical point at $H = 20\text{T}$, and $T = 4\text{K}$. The presence of three low-temperature transitions at $T_{N1} = 4.7\text{K}$, $T_{N2} = 3.3\text{K}$, and $T_{N3} = 2.3\text{K}$ clearly indicated a complex interaction topology: Between T_{N3} and T_{N2} , β -TeVO₄ reveals an enigmatic stripe-like spin texture, whereas between T_{N2} and T_{N1} a spin-density-wave (SDW) phase akin to the field-induced SDW phase in LiCuVO₄ has been proposed. The nature of different phases and regions is far from completely understood, and will be further investigated by ¹²⁵Te NMR.

- [1] F. Weickert, N. Harrison, B. L. Scott, M. Jaime, A. Leitmäe, I. Heinmaa, R. Stern, O. Janson, H. Berger, H. Rosner, and A. A. Tsirlin, "Magnetic anisotropy in the frustrated spin-chain compound β -TeVO₄", *Phys. Rev. B* **94** (2016), 10.1103/PhysRevB.94.064403.

*Corresponding author: raivo.stern@kbfi.ee

Multi-order Raman scattering in orthorhombic manganites

N.N. Kovaleva*¹

¹*Lebedev Physical Institute, Russian Academy of Sciences, 119991 Moscow, Russia*

The multi-order Raman scattering is studied up to a fourth order for a detwinned LaMnO_3 crystal. Based on a comprehensive data analysis of the polarization-dependent Raman spectra, we show that the anomalous features in the multi-order scattering could be the sidebands on the low-energy mode at 25 cm^{-1} . The sidebands are dominated by the oxygen contribution to the phonon density-of-states, however, there is an admixture of an additional component, which may arise from strong coupling between the low-energy electronic motion and the vibrational modes. The results are juxtaposed to the Raman scattering spectra observed in other crystals of orthorhombic rare-earth (RE) manganites. The origin of the low-energy mode at 25 cm^{-1} and the mechanism of multi-order Raman scattering are analyzed.

*Corresponding author: nkovaleva@lebedev.ru

Transient localization of gap modes in crystals of NaI at high temperature: insight and questions from wavelet analysis

A. Riviere¹, M. Assani¹, D. Colognesi², S. Lepri², and F. Piazza*^{1,3}

¹Université d'Orléans, Pôle de Physique et Sciences de l'Ingénieur,
Rue de Chartres, B.P. 6759, 45067 Orléans cedex 2, France

²Istituto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche,
Via Madonna del Piano 10, I-50019, Sesto Fiorentino (Italy)

³Centre de Biophysique Moléculaire (CBM), CNRS UPR4301, Rue C. Sadron, 45071, Orléans, France

In this talk we report the results of extensive NVE molecular dynamics simulations of NaI crystals with realistic interatomic potentials. We use a wavelet-based original method to study energy localization in the time-frequency plane. Our results show clearly that soft nonlinear vibrational components appear for temperatures greater than about 400 K in the vibrations of light atoms. These manifest themselves as intermittent bursts of energy in the gap of average duration of the order of 10 ps (see Fig. 1). The question arises as whether such self-localizing vibrations are thermally activated discrete breathers (DB). Two observations seem to contradict this interpretation. First, we systematically fail in detecting simultaneous energy bursts in the gap in the wavelet spectra of neighboring I ions. Second, a statistical analysis of the burst excitation rate as a function of temperature (measured from the statistics of the inter-burst excitation times) does not appear to be consistent with the expected presence of an energy excitation threshold for DB modes. The question as to the physical nature of the observed soft short-lived gap modes remains open.

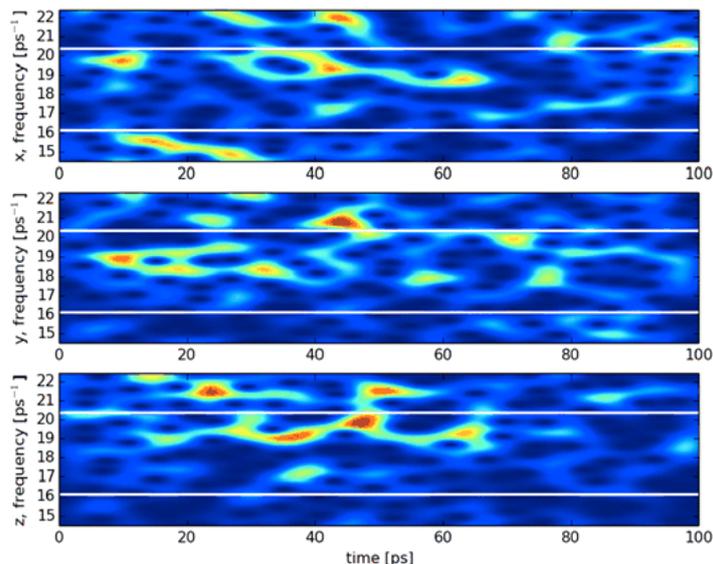


Figure 1: Wavelet analysis of the vibrations of a Na ion in a NaI crystal at $T = 600$ K. Close-up in the spectral region of the gap (region comprised between the two white lines) showing bursts of energy localization with a duration of the order of 10 ps.

*Corresponding author: Francesco.Piazza@cnrs-orleans.fr

Delocalized vibrational modes in graphene: second harmonic generation and negative pressure

E.A. Korznikova*¹, S.A. Shcherbinin², D.S. Ryabov², G.M. Chechin², and S.V. Dmitriev^{1,3}

¹*Institute for Metals Superplasticity Problems of RAS, Khalturin St. 39, 450001 Ufa, Russia*

²*Southern Federal University, Institute of Physics, Stachki Ave., 194, Rostov-on-Don 344090, Russia*

³*National Research Tomsk State University, Lenin Avenue 36, 634050 Tomsk, Russia*

With the help of molecular dynamics simulations, delocalized vibrational modes (DVM) in graphene are analyzed. Such modes are dictated by the lattice symmetry, they are exact solutions to the atomic equations of motion, regardless the employed interatomic potential and for any mode amplitude. In this study, only one- and two-component DVM are analyzed, they are reducible to the dynamical systems with one and two degrees of freedom, respectively. There exist 4 one-component and 12 two-component DVM with in-plane atomic displacements. Any two-component mode includes a one-component mode. If the amplitudes of the modes constituting a two-component mode are properly chosen, periodic in time vibrations are observed at frequencies ω and 2ω , i.e., second harmonic generation takes place. For particular DVM, the higher harmonic can have frequency nearly two times larger than the maximal frequency of the phonon spectrum of graphene. Excitation of some of DVM results in the appearance of negative in-plane pressure in graphene. This counterintuitive result is explained by the rotational motion of carbon hexagons. Our results contribute to the understanding of nonlinear dynamics of graphene lattice.

*Corresponding author: elena.a.korznikova@gmail.com

Effect of discrete breathers on energy transport in 1D nonlinear lattices

Sergey V. Dmitriev^{*1,2}, Daxing Xiong³, and Danial Saadatmand⁴

¹*Institute for Metals Superplasticity Problems of RAS, Khalturin St. 39, 450001 Ufa, Russia*

²*National Research Tomsk State University, Lenin Avenue 36, 634050 Tomsk, Russia*

³*Department of Physics, Fuzhou University, Fuzhou 350108, Fujian, China*

⁴*Department of Physics, University of Sistan and Baluchestan, Zahedan, Iran*

Anomalous (non-Fourier) heat transport is no longer just a theoretical issue since it has been observed experimentally in a number of low-dimensional nanomaterials, such as SiGe nanowires, carbon nanotubes, and others. To understand these anomalous behaviors, exploring the microscopic origin of normal (Fourier) heat transport is a fascinating theoretical topic. However, this issue has not yet been fully understood even for one-dimensional (1D) model chains, in spite of a great amount of thorough studies done to date. From those studies, it has been widely accepted that the conservation of momentum is a key ingredient to induce anomalous heat transport, while momentum-nonconserving systems usually support normal heat transport where Fourier's law is valid. But if the nonconservation of momentum is the reason, what is the underlying microscopic mechanism for the observed normal heat transport? Here we carefully revisit a typical 1D momentum-nonconserving ϕ^4 model, and we present evidence that the mobile discrete breathers, or, in other words, the moving intrinsic localized modes with frequency components above the linear phonon band, can be responsible for that.

Power of the energy source in the form of single ac driven particles is calculated numerically for different amplitudes A and frequencies ω the linear phonon band. The results for the on-site potentials with hard and soft anharmonicity types are compared. For the hard-type anharmonicity, it is shown that when the driving frequency is close to (far from) the edge of the phonon band, the power of the energy source normalized to A^2 increases (decreases) with increasing amplitude. In contrast, for the soft-type anharmonicity, the normalized power of the energy source increases (decreases) with increasing A when the driving frequency is close to (far from) the lower edge of the phonon band. Our further demonstrations indicate that, in the case of hard (soft) anharmonicity, the chain can support movable discrete breathers (DBs) with frequencies above (below) the phonon band. It is the energy source quasi-periodically emitting moving DBs in the regime with driving frequency close to the DBs frequency, that induces the increase of the power. Therefore, our results here support the mechanism that the moving DBs can assist energy transfer from the ac driven particle to the chain.

*Corresponding author: dmitriev.sergey.v@gmail.com

Spontaneous currents in spatially inhomogeneous $s + is$ superconductors

M. Silaev*¹

¹*Department of Physics and Nanoscience Center, University of Jyväskylä, P.O. Box 35 (YFL), FI-40014 University of Jyväskylä, Finland*

Recently a lot of attention has been focused on the broken time-reversal symmetry states in multiband superconductors. In particular, two candidate states, namely $s + is$ and $s + id$ have been proposed theoretically that in the $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ system, where the signatures of spontaneous currents have been observed experimentally [1]. Here I discuss theoretically that such currents can be generated due to the spatial inhomogeneities both in the $s + is$ and $s + id$ states. I show that due to the c -axis anisotropy these states yield spontaneous currents of the same magnitude.

- [1] V. Grinenko et al., “Superconductivity with broken time-reversal symmetry in ion-irradiated $\text{Ba}_{0.27}\text{K}_{0.73}\text{Fe}_2\text{As}_2$ single crystals”, *Phys. Rev. B* **95**, 214511 (2017).

*Corresponding author: mikesilaev@gmail.com

Quasiparticle current-voltage characteristics for break junctions involving d -wave superconductors unstable against charge-density-wave formation

A.M. Gabovich*¹, A.I. Voitenko¹, Mai Suan Li², H. Szymczak², and T. Ekino³

¹*Institute of Physics, National Academy of Sciences of Ukraine, 46, Nauka Ave., Kyiv 03680, Ukraine*

²*Institute of Physics, PL-02-668, Warsaw, Poland*

³*Hiroshima University, Graduate School of Integrated Arts and Sciences, Higashi-Hiroshima, 739-8521, Japan*

Tunnel conductance voltage, V , dependences (CVCs), $G(V)$, is calculated for break junctions (BJs) involving layered d -wave superconductors partially gapped by charge density waves (CDWs). The quasiparticle current is assumed to flow in the ab -plane of electrodes. The influence of CDWs is analyzed by comparison of the CVCs for CDW d -wave superconductors with CVCs calculated for BJ made up of pure superconductors. The main CDW-effects were found to be the appearance of new CVC peculiarities and the loss of CVC symmetry with respect to the V -sign. Tunnel directionality is extremely important in this case as well. In particular, the orientation of electrodes with respect to the current channel becomes very important. As a result, $G(V)$ can acquire a large variety of forms similar to those for tunnel junctions between superconductors with s -wave, d -wave, and mixed symmetry of their order parameters but distorted by the CDW involvement. The diversity of peculiarities is especially striking at finite temperatures. In the case of BJ made up of pure d -wave superconductors, the resulting CVC can include a two-peak gap-driven structure. The apparent features of either s - or d -symmetry strongly depend on the electrode orientation. The results were compared with the experimental BJ data for a number of high- T_c oxides. It was shown that the large variety of the observed current-voltage characteristics can be interpreted in the framework of our approach. Thus, quasiparticle tunnel currents in the ab -plane can be used as an effective tool to detect CDWs competing with superconductivity in cuprates or other layered superconductors.

*Corresponding author: alexander.gabovich@gmail.com

Nonlinear atomic vibrations in strained graphene monolayer: bushes of nonlinear normal modes

George Chechin*¹, Denis Ryabov¹, and Stepan Shcherbinin¹

¹*Institute of Physics, Southern Federal University, Stachki ave. 194, Rostov-on-Don, 344090, Russia*

We discuss some type of the strong anharmonic atomic vibrations of two-dimensional graphene crystal lattice, which represent symmetry-determined nonlinear normal modes by Rosenberg (NNMs) and their bushes. They represent *exact* solutions to nonlinear dynamical equations above the traditional harmonic approximation for N -particle Hamiltonian systems with discrete symmetry. The general theory of bushes of NNMs was developed in [1-3]. Bushes of vibrational modes in physical systems with different point and space symmetries were studied in the series of our previous works.

Every bush is characterized by a subgroup $G_j \subset G_0$ of the symmetry group G_0 of dynamical system in its equilibrium state (or a subgroup of its Hamiltonian). The possibility of a given bush to exist as exact dynamical regime is provided by some symmetry-related selection rules for excitation transfer between modes of different symmetry. In particular, a vibrational mode with higher symmetry cannot excite any mode with lower symmetry: excitation transfers from a given mode to the modes with higher symmetry group, *independently* of the specific type of interparticle interactions in the considered physical system.

Construction of the bushes of NNMs can be performed with the aid of the specific group-theoretical methods based on the apparatus of irreducible representations of the symmetry groups. Each bush represents a full collection of nonlinear normal modes, which are connected by “force” interactions, and the number of these modes (m) is the dimension of the given bush. It is essential that bushes with small dimensions (for example, with $m = 1, 2, 3, 4, \dots$) can be excited in many physical systems with discrete symmetry. One-dimensional bushes ($m = 1$) describe time-periodical motion while bushes with $m > 1$ describe quasi-periodical motion with m basis frequencies in the Fourier spectrum.

Every bush represents a dynamical object since amplitudes of these modes change during the time evolution. It can be considered as an individual Hamiltonian system, whose dimension is less than the whole dimension of the considered system. The energy of the initial excitation turns out to be trapped in the given bush. Stability of the given bush takes place, if the collection of its modes is conserved in time. If the bush with the symmetry group G_j loses stability, when we increase the energy of initial excitation, it transforms into another bush with larger dimension and with lower symmetry group $\tilde{G}_j \subset G_j$.

In the present report, we discuss group-theoretical results on the small-dimensional vibrational bushes in graphene (some previous results were published in our papers [4,5]). All low-dimensional bushes in graphene have been found. It occurs that there are 4 one-dimensional, 14 two-dimensional, 1 three-dimensional and 6 four-dimensional bushes can exist in graphene. We present displacement patterns of the modes entering above bushes and discuss the behavior of their modes in time obtained with the aid of *ab initio* simulations based on the density functional theory.

- [1] V.P. Sakhnenko, G.M. Chechin. *Dokl.Akad.Nauk* **330**, 308 (1993);
V.P. Sakhnenko, G.M. Chechin. *Phys. Dokl.* **38**, 219 (1993).
- [2] G.M. Chechin, V.P. Sakhnenko. *Physica D* **117**, 43 (1998).
- [3] G.M. Chechin, K.G. Zhukov. *Phys. Rev. E* **73**, 36216 (2006).
- [4] G.M. Chechin, D.S. Ryabov, S.A. Shcherbinin. *Letters on materials* **6**, 9 (2016).
- [5] G.M. Chechin, D.S. Ryabov, S.A. Shcherbinin. *Letters on materials* **7**, 367 (2017).

*Corresponding author: gchechin@gmail.com

Nonlocal breathers as possible energy carriers in secondary tracks in muscovite

J.F.R. Archilla*¹, Y. Doi², and M. Kimura³

¹*Group of Nonlinear Physics, Universidad de Sevilla, ETSI Informática,
Avda Reina Mercedes s/n, 41012-Sevilla, Spain*

²*Department of Adaptive Machine Systems, Graduate School of Engineering, Osaka University
2-1 Yamadaoka, Suita, Osaka 565-0871, Japan*

³*Department of Electrical Engineering, Kyoto University Katsura, Nishikyo-ku, Kyoto 615-8510, Japan*

The experimental existence of quodons, that is, nonlinear excitation that leave fossil tracks in mica muscovite, was obtained in 2007 [1]. Many tracks were initiated by the recoil of ⁴⁰K and the analysis of its decay modes [2] together with the study of the tracks suggested that quodons have charge [3] and that different kinds of quodons with different charge states existed [4]. The transport of charge by quodons was recently demonstrated experimentally [5]. Fossil tracks show that primary tracks are very energetic while secondary ones are much more weak [6]. Kinks were shown to have the appropriate energy [7]. Kinks, double kinks and nanopterons were shown to exist in a realistic model[8].

In this presentation we show that in the same model also there exists an array of breathers with small energies which could correspond to quodons for secondary tracks. Exact moving breathers can be obtained but they are coupled to a plane wave and are called tail-breathers or nonlocal breathers. Their significance as proper physical solutions is analyzed. Their structure also poses theoretical questions as the plane wave and the breather core travel in opposite directions. An explanation based in the description of the system in the extended zone is proposed [9].

The authors JFRA wish to thank project FIS2015-65998-C2-2-P from MINECO and grant 2017/FQM-280 from Junta de Andalucía, Spain and a travel grant from the VI PPIT-US of Universidad de Sevilla, Spain. YD acknowledges the support of JSPS KAKENHI Grant Number 16K05041.

- [1] F.M. Russell, J.C. Eilbeck, "Evidence for moving breathers in a layered crystal insulator at 300 K", *EPL* **78**(1), 10004 (2007).
- [2] J.F.R. Archilla, Yu. A. Kosevich, N. Jiménez, V.J. Sánchez-Morcillo, L.M. García-Raffi, "A Supersonic crowdion in mica", in J.F.R. Archilla, et al, editors, *Quodons in Mica*, Springer Ser. Mater. Sci., **221**, 69-96 (2015).
- [3] F.M. Russell, "Tracks in mica, 50 years later", in J.F.R. Archilla, et al, editors, *Quodons in Mica*, Springer Ser. Mater. Sci., **221**, 3-33 (2015).
- [4] J.F.R. Archilla, F.M. Russell, "On the charge of quodons", *Lett. Mater.* **6**(1),3-8 (2016).
- [5] F.M. Russell, J.F.R. Archilla, F. Frutos, S. Medina-Carrasco "Infinite charge mobility in muscovite at 300K", *Europhys. Lett.*, **120**(4) 46001 (2017).
- [6] F.M. Russell, "Transport Properties of Quodons in Muscovite and Prediction of Hyper-Conductivity", in JFR Archilla et al., Editors, *Nonlinear Systems*, Vol. 2. Springer, pp. 241-260 (2018).
- [7] J.F.R. Archilla, Yu. A. Kosevich, N. Jiménez, V.J. Sánchez-Morcillo, L.M. García-Raffi, "Ultradiscrete kinks with supersonic speed in a layered crystal with realistic potentials", *Phys. Rev. E* **91**(2), 022912 (2015).
- [8] J.F.R. Archilla, Y. Zolotaryuk, Yu. A. Kosevich, Y Doi, "Nonlinear waves in a model for silicate layers", Submitted.
- [9] J.F.R. Archilla, Y. Doi. " Moving breathers in a model for a layered crystal with realistic potentials", In preparation.

*Corresponding author: archilla@us.es

Phase dynamics of nonlinear localized excitations in weakly coupled anharmonic chains and analogy between periodic tunneling of classical and quantum objects

Yu.A. Kosevich*¹

¹*Semenov Institute of Chemical Physics RAS, 4 Kosygin str., 119991 Moscow, Russia*

We present a brief survey of the phase-coherent dynamics of discrete breathers (intrinsic localized modes) and dark lattice solitons in a system of two weakly coupled nonlinear chains and its comparison with periodic tunneling of a quantum particle in a double-well potential and with macroscopic quantum tunneling of two weakly linked Bose-Einstein condensates. We consider the dynamics of relative phase of classical-tunneling intrinsic localized mode and dark lattice soliton in two weakly coupled nonlinear chains. The dynamics of the relative phase in the $\pi/2$ tunneling mode of the dark lattice soliton coincides with the experimentally observed dynamics of the relative phase of repulsive quantum particles, periodically co-tunneling in a double-well potential [1]. The observed coincidence demonstrates the profound analogy between the dynamics of classical localized excitations in two weakly coupled nonlinear chains and tunneling dynamics of quantum objects in the double-well potential. We show that in both $\pi/2$ and winding tunneling modes, the relative phase experiences periodic jumps by π in the instants of complete depopulation of one of the weakly coupled chains or potential wells. The connection of the features of the observed phase dynamics with the uncertainty principle is discussed.

- [1] S. Fölling, S. Trotzky, P. Cheinet, M. Feld, R. Saers, A. Widera, T. Müller, I. Bloch, “Direct observation of second-order atom tunneling”, *Nature* **448**, 1029-1033 (2007).

*Corresponding author: yukosevich@gmail.com

Discrete breathers in hydrogenated metals: atomistic simulations and applications to the rate theory

V. Dubinko^{*1,2}, D. Laptev^{2,3}, D. Terentyev⁴, and K. Irwin²

¹NSC "Kharkov Institute of Physics and Technology", Kharkov 61108, Ukraine

²Quantum Gravity Research, Los Angeles, CA 90066, USA

³B. Verkin Institute for Low Temperature Physics and Engineering, Kharkov 61103, Ukraine

³SCK-CEN, Nuclear Materials Science Institute, Mol 2400, Belgium

Hydrogenation is a chemical reaction between molecular hydrogen and another compound or element, usually in the presence of a *catalyst* such as *nickel* or *palladium*. There is no single theory of catalysis, but only a series of principles to interpret the underlying processes. An important parameter of the reaction kinetics is the *activation energy*, i.e. the energy required to overcome the reaction barrier. The lower is the activation energy, the faster the reaction rate, and so a catalyst may be thought to reduce somehow the activation energy. Dubinko et al [1-4] have shown that in a crystalline matrix, the activation energy may be reduced at some sites due to a special class of localized anharmonic vibrations of atoms, known also as *intrinsic localized modes* or *discrete breathers* (DBs).

We present atomistic simulations of DBs in nickel, palladium and their hydrides. Large amplitude atomic motion in DBs may result in time-periodic driving of adjacent potential wells occupied by hydrogen ions (protons or deuterons). This driving has been shown to result in the increase of amplitude and energy of zero-point vibrations and in broadening of the wave packet [5, 6]. In this context, we present numerical solution of Schrodinger equation for a particle in a non-stationary double well potential, which is driven time-periodically imitating the action of a DB. We show that the rate of tunneling of the particle through the potential barrier separating the wells is drastically enhanced by the driving with a resonant frequency ranging from ω_0 to $2\omega_0$, where ω_0 is the eigenfrequency of the potential well. The effect increases strongly with increasing amplitude of the driving. These results support the concept of DB mediated catalysis and extend it to low temperatures where quantum tunneling prevails over thermal activation controlling the reaction rates in solids.

- [1] V. Dubinko, P. Selyshchev, J. Archilla, "Reaction-rate theory with account of the crystal anharmonicity", *Phys. Rev. E* **83**, No 4 (2011), DOI: 10.1103/PhysRevE.83.041124.
- [2] V. Dubinko, F. Piazza, "On the role of disorder in catalysis driven by discrete breathers", *Letters on Materials* **4** (4), 273-278 (2014).
- [3] V. Dubinko, A. Dubinko, "Modification of reaction rates under irradiation of crystalline solids: contribution from intrinsic localized modes", *Nuclear Inst. and Methods in Physics Research*, B **303**, 133-135 (2013).
- [4] D. Terentyev, A. Dubinko, V. Dubinko, S. Dmitriev, E. Zhurkin, "Interaction of discrete breathers with primary lattice defects in bcc Fe", *Modelling Simul. Mater. Sci. Eng.* **23**, 085007-13 (2015).
- [5] V. I. Dubinko, D. V. Laptev, Chemical and nuclear catalysis driven by localized anharmonic vibrations, *Letters on Materials* **6**, 16-21, (2016).
- [6] V. I. Dubinko, D. V. Laptev, A. S. Mazmanishvili, J. F. R. Archilla, "Quantum dynamics of wave packets in a nonstationary parabolic potential and the Kramers escape rate theory", *J. Micromechanics and Molecular Physics*, **1**, 650010-1-12 (2016).

*Corresponding author: vdubinko@hotmail.com

Out of plane s-orbital contributions investigated by resonant photoemission on (Bi,Pb)2201 and (Bi,Pb)2212

C. Janowitz*¹ and D. Schmei er²

¹*Institut f ur Physik, Humboldt-Universit t zu Berlin, Newtonstr. 15, 12489 Berlin, Germany*

²*Angewandte Physik-Sensorik, BTU Cottbus-Senftenberg, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany*

It is common wisdom to assume that in high-temperature superconductors with layered crystal structure the copper-oxygen planes dominate the electronic properties around the Fermi energy. As a consequence, out-of-plane contributions are often neglected in the description of these materials. Even more strong correlation effects inherent to models with reduced dimensionality like the two-dimensional Hubbard model are often regarded to account for the essential physics.

However the importance of out of plane degrees of freedom was highlighted recently. In a pump-probe experiment on $\text{YBa}_2\text{Cu}_2\text{O}_{6+\delta}$, a perpendicular transient state with highly coherent transport resembling a superconducting state up to RT was created by excitation with mid-infrared optical pulses, tuned to the resonant frequency of apical oxygen vibrations [1]. It highlights the importance of modulated lattice and electronic properties out-of-plane. Here we report on a resonant photoemission study of $\text{Pb}_{0.4}\text{Bi}_{1.6}\text{Sr}_{2.0}\text{CaCu}_2\text{O}_8$ ((Pb,Bi)-2212) and $\text{Pb}_{0.6}\text{Bi}_{1.4}\text{Sr}_{1.5}\text{La}_{0.5}\text{CuO}_6$ ((Pb,Bi)-2201)) single crystals to unravel the resonant decay mechanisms at the Cu2p absorption edge [2]. We find evidence for a pronounced polarization dependence caused by two different Auger processes for in-plane and out-of-plane orientations. We deduce that the lowest energy valence state - which is involved in the two Auger processes - consists of 3-dim contributions by admixed out-of-plane Sr, Bi, and O2p states. It also suggests that the doping induced charge density is dynamic fluctuating within the Cu-O plane and spills out perpendicular to it. This suggests that out-of-plane electronic degrees of freedom needs to be included in future consistent theoretical models of these materials.

- [1] S. Kaiser, C.R. Hunt, D. Nicoletti, W. Hu, I. Gierz, H.Y.Liu, M. Le Tacon, T. Loew, D. Haug, B. Keimer and A. Cavallieri, *Phys. Rev. B* **89**, 184516 (2014).
[2] C. Janowitz, D. Schmei er, *Supercond. Sci. Technol.* **31**, 045006 (2018)

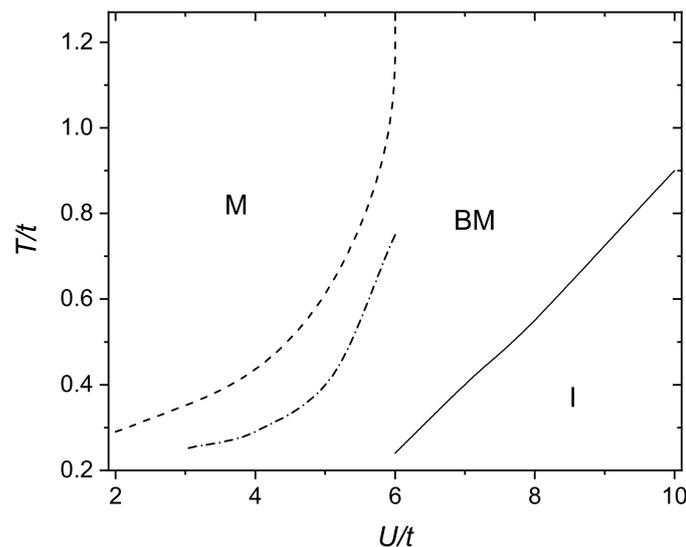
*Corresponding author: Janowitz@physik.hu-berlin.de

Influence of spin and charge fluctuations on spectra of the two-dimensional Hubbard model

A. Sherman*¹

¹*Institute of Physics, University of Tartu, W. Ostwaldi Str 1, 50411 Tartu, Estonia*

The influence of spin and charge fluctuations on spectra of the two-dimensional fermionic Hubbard model is considered using the strong coupling diagram technique. Infinite sequences of diagrams containing ladder inserts, which describe the interaction of electrons with these fluctuations, are summed, and obtained equations are self-consistently solved for the ranges of Hubbard repulsions $2t \leq U \leq 10t$, temperatures $0.2t \lesssim T \lesssim t$ and electron concentrations $0.7 \lesssim \bar{n} \leq 1$ with t the intersite hopping constant. For all considered U the system exhibits a transition to the long-range antiferromagnetic order at $T_{AF} \approx 0.2t$. At the same time no indication of charge ordering is observed. Obtained solutions agree satisfactorily with Monte Carlo data and satisfy moments sum rules. The phase diagram of the model is shown in the figure. The dashed curve separates metallic (M) solutions. If only short-range fluctuations are allowed for the remaining part of the U - T plane is occupied by insulating (I) solutions. Taking into account long-range fluctuations leads to strengthening the tails of maxima that transform a part of insulating solutions into bad-metal (BM) states. For low T , obtained results allow us to trace the gradual transition from the regime of strong correlations with the pronounced four-band structure and well-defined Mott gap for $U \gtrsim 6t$ to the Slater regime of weak correlations with the spectral intensity having a dip along the boundary of the magnetic Brillouin zone due to an antiferromagnetic ordering for $U \lesssim 3t$. For $T \approx T_{AF}$ and $U \gtrsim 7t$ doping leads to the occurrence of a pseudogap near the Fermi level, which is a consequence of the splitting out of a narrow band from a Hubbard subband.



*Corresponding author: alekseis@ut.ee

Influence of short-range correlations on the band structure of doped Mott insulators

V.I. Kuz'min*¹, S.V. Nikolaev^{1,2}, and S.G. Ovchinnikov^{1,2}

¹*Kirensky Institute of Physics, Federal Research Center KSC SB RAS, Krasnoyarsk, 660036 Russia*

²*Siberian Federal University, Krasnoyarsk, 660041 Russia*

In the present work the electronic spectral function is calculated within the Hubbard and Hubbard-Holstein models in the framework of cluster perturbation theory (CPT)[1] using X-operator technique[2] based on exact full diagonalization of 3x3 and 2x2 clusters. We use exact diagonalization with account for a full basis of cluster eigenstates as a cluster solver, unlike most CPT calculations within the Hubbard model, which use the ground state Lanczos method to obtain clusters Green's function. This gives us a possibility to calculate the electronic Green's function without an artificial Lorentzian broadening. Thus, fine properties of quasiparticle subbands are easily accessed. Our data obtained within CPT along with the analysis of intracuster correlation functions obtained on 3x3 and 4x4 clusters allows investigating the effect of short-range correlations stemming from local Coulomb and electron-phonon interactions on the electronic structure. We obtain different anomalous spectral features of doped Mott insulators, such as Fermi-arcs, kinks and waterfalls[3-5]. Also, features similar to the electron-like Fermi-pockets of cuprates at hole doping $p \sim 0.1$ [6] are obtained without *ad hoc* introducing a charge density wave order parameter. Within the Hubbard-Holstein model we observe that splitting of fermion bands can cause low-energy kink-like features at moderate phonon frequency and low electron-phonon interaction.

The reported study was funded by RFBR according to the research project No. 18-32-00256 (all the results except correlation functions calculated using 4x4 clusters). The authors are grateful to the Presidium RAS program No. 12 "Fundamental problems of high temperature superconductivity", "BASIS" Foundation for Development of Theoretical Physics and Mathematics, and Russian Foundation for Basic Research (grant 16-02-00098), Government of Krasnoyarsk Territory, Krasnoyarsk Region Science and Technology Support Fund to the research project 18-42-243004.

- [1] D. Senechal, D. Perez, and M. Pioro-Ladriere, *Phys. Rev. Lett.* **84**, 522 (2000).
- [2] S. V. Nikolaev and S. G. Ovchinnikov, *Journal of Experimental and Theoretical Physics* **111**, 635 (2010).
- [3] A. Damascelli, Z. Hussain, and Z.-X. Shen, *Rev. Mod. Phys.* **75**, 473 (2003).
- [4] J. C. Campuzano et al., *Phys. Rev. Lett.* **83**, 3709 (1999).
- [5] J. Graf et al., *Phys. Rev. Lett.* **98**, 067004 (2007).
- [6] D. LeBoeuf et al., *Nature* (London) **450**, 533 (2007).

*Corresponding author: kuz@iph.krasn.ru

Boson magnetism in strongly correlated cold atom system

A.M. Belemuk^{1,2}, N.M. Chtchelkatchev^{*1,2,3}, A.V. Mikheyenkov^{1,2}, and K.I. Kugel^{4,5,6}

¹*Institute for High Pressure Physics, Moscow (Troitsk) 108840, Russia*

²*Moscow Institute of Physics and Technology (State University), Moscow 141700, Russia*

³*L.D. Landau Institute for Theoretical Physics, Moscow 119334, Russia*

⁴*National Research Center "Kurchatov Institute", Moscow 123182, Russia*

⁵*Institute for Theoretical and Applied Electrodynamics, Moscow 125412, Russia*

⁶*National Research University Higher School of Economics, Moscow 101000, Russia*

Quantum state of cold atoms in optical lattices in the Mott insulator regime when hopping is suppressed is basically governed by density-density and (pseudo)spin-(pseudo)spin interactions, U_0 and U_s , that, in turn, might be tuned *in situ*, contrary to strongly correlated electrons in solids [1]. We show, on the same unified footing, for a number of cold-atom systems, vector Fermions or Bosons, how tuning U_0 and U_s drives the sequence of quantum phase transitions (QPT) that involve (pseudo)spin state and particle ordering. These QPT originate from competing interactions.

As an example, we analyze possible types of ordering in a boson–fermion model. The Hamiltonian is inherently related to the Bose–Hubbard model for vector two-species bosons in optical lattices. We show that such model can be reduced to the Kugel–Khomskii type spin–pseudospin model, but in contrast to the usual version of the latter model, we are dealing here with the case of spin $S=1$ and pseudospin $1/2$. We show that the interplay of spin and pseudospin degrees of freedom leads to a rather nontrivial magnetic phase diagram including spin-nematic configurations. Tuning the spin-channel interaction parameter U_s gives rise to quantum phase transitions. We find that the ground state of the system always has the pseudospin domain structure. On the other hand, the sign change of U_s switches the spin arrangement of the ground state within domains from ferro to antiferromagnetic. Finally, we revisit spin (pseudospin)- $1/2$ Kugel–Khomskii model [2] and see inverse picture of phase transitions.

We present new results for this system also when in addition to the standard parameters characterizing it, we are dealing with the “degree of atomic nonidentity”, manifesting itself in the difference of tunneling amplitudes and on-site Coulomb interactions. We obtain a cascade of quantum phase transitions occurring with the increase in the degree of atomic nonidentity. While in the system of nearly identical vector bosons, only one phase transition between two phases occurs with the evolution of the interparticle interaction, atom nonidentity increases the number of possible phases to six, while the resulting phase diagrams are so nontrivial that we can speculate about their evolution from the images similar to the “J.-Miro-like paintings” to “K.-Malewicz-like” ones [3-4].

[1] O. Dutta, M. Gajda, P. Hauke, et al, *Rep. Prog. Phys.* **78**, 066001 (2015).

[2] K.I. Kugel, D.I. Khomskii, *Sov. Phys. - Uspekhi* **25**, 231 (1982).

[3] A.M. Belemuk, N.M. Chtchelkatchev, A.V. Mikheyenkov, and K.I. Kugel, *Phys. Rev. B* **96**, 094435 (2017).

[4] A.M. Belemuk, N.M. Chtchelkatchev, A.V. Mikheyenkov, and K.I. Kugel, *arxiv* 1802.06236, 2017.

*Corresponding author: nms@itp.ac.ru

Stability of the superconducting d -wave pairing towards the Coulomb repulsions in cuprate superconductors

V.V. Val'kov¹, D.M. Dzebisashvili^{1,2}, M.M. Korovushkin*¹, and A.F. Barabanov³

¹*Kirensky Institute of Physics, Federal Research Center KSC SB RAS, 660036 Krasnoyarsk, Russia*

²*Siberian State University of Science and Technology, 660037 Krasnoyarsk, Russia*

³*Vereshchagin Institute for High Pressure Physics, 108840 Troitsk, Moscow, Russia*

It is known that formation of physical properties of high-temperature cuprate superconductors (HTCS) takes place at the strong interplay between spin and charge degrees of freedom. In particular, the strong spin-fermion correlations underlie the formation of the spin-polaron quasiparticles [1]. The theory based on the spin-polaron concept allows one to describe correctly a number of important features of the spectral properties of HTCS in the normal phase [2]. An important factor confirming the promise of this concept is the occurrence of the Cooper instability in the ensemble of the spin-polaron quasiparticles for the actual d -wave pairing [3] and critical temperatures corresponding to the experimental data.

Recently, the spin-polaron concept acquired special significance, since it allowed one to solve a long-standing problem in HTSC theory. This problem related to the fact that the Cooper instability in the d -wave superconducting channel in cuprate superconductors is completely suppressed, as soon as the Coulomb repulsion of holes located at the nearest sites is taken into account. This problem is clearly manifested, for example, in the framework of the Hubbard model or the t - J model on a simple square lattice. In our recent papers [4,5], it was shown that the d -wave channel of Cooper pairing is insensitive towards the strong Coulomb repulsion of holes located at the nearest oxygen ions if the real structure of the CuO_2 plane, as well as the strong spin-fermion coupling between localized spins on copper ions and holes on oxygen ions are taken into account. The analysis showed that only the superconducting d -wave pairing is implemented at whole region of doping, whereas the non-trivial solutions of the self-consistent equations for the superconducting s -wave pairing are absent.

The work was supported by the program of the Presidium of the Russian Academy of Sciences No. 12 "Fundamental problems of high-temperature superconductivity", the Russian Foundation for Basic Research (RFBR) and partly by the Government of Krasnoyarsk Region and the Krasnoyarsk Region Science and Technology Support Fund (projects no. 18-42-243002). The work of A.F.B. was funded by RFBR (project no. 16-02-00304). The work of M.M.K. was supported by a grant of the President of the Russian Federation (project MK-1398.2017.2).

[1] A.F. Barabanov, A.V. Mikheenkoy, A.M. Belemuk, *JETP Lett.* **47**, 107 (2002).

[2] V.V. Val'kov, D.M. Dzebisashvili, A.F. Barabanov, *JETP Lett.* **98**, 528 (2013).

[3] V.V. Val'kov, D.M. Dzebisashvili, A.F. Barabanov, *Phys. Lett. A* **379**, 421 (2015).

[4] V.V. Val'kov, D.M. Dzebisashvili, M.M. Korovushkin, A.F. Barabanov, *JETP Lett.* **103**, 385 (2016).

[5] V.V. Val'kov, D.M. Dzebisashvili, M.M. Korovushkin, A.F. Barabanov, *JETP* **125**, 810 (2017).

*Corresponding author: kmax@iph.krasn.ru

Effects of chirality and strong electron localization in a crystalline yttrium oxyhydride

E. Strugovshchikov^{*1}, A. Pishtshev¹, and S. Karazhanov²

¹*Institute of Physics, University of Tartu, W.Ostwaldi Str 1, 50411 Tartu, Estonia*

²*Department for Solar Energy, Institute for Energy Technology, Kjeller, Norway*

In this contribution, we present the recent theoretical results of our research work on functionality of yttrium oxyhydride (Y-H-O) materials. The main objective is to understand from first-principles how oxygen as active chemical element of the inorganic ternary compound governs the interplay of the local charge geometries and short-range covalency, and provides the global lattice stability via the possible structural transformations. The fundamental aspect of our work is that we determined a structural trend driven by the combination of metal-oxygen and oxygen-hydrogen interactions. The stability of all active chemical interactions follows from the cooperative effect which causes the spatial separation of the Y-H, Y-O, and O-H bonding channels. We showed that this effect underlies a number of structural and electron features. The two main of these features are the chirality of the inorganic crystal structure and the strong localization of valence charge densities. The localization corresponds to a specific charge ordering which is established via the helical patterns of atoms in the lattice. The results allowed us to predict unusual ferroelectric and optical properties of the material.

^{*}Corresponding author: evgenii.strugovshchikov@ut.ee

The similarity of vibronic mechanisms during dimerization and reverse recovery of the aromatic compounds

V. Krasnenko*¹

¹*Institute of Physics, University of Tartu, W. Ostwaldi Str 1, 50411, Tartu, Estonia*

The vibronic interactions may play a significant role in the covalent bonds formation and breaking between adjacent aromatic compounds. The recent investigations [1-4] have predicted the possibility of covalent dimerization of benzene molecules (bi-benzene), covalently conjoined structures of benzene molecule and graphene sheet (graphene can consider as an indefinitely large aromatic molecule) indicating on the similar vibronic mechanism of their formation.

The existence of the above-described structures is confirmed by the presence of dimerized thymine bases in deoxyribonucleic acid (DNA), which may lead to skin cancer (see, e.g. [5-7]). Moreover, according to performed research, the most energetically favorable of the predicted structures of bi-benzene, benzene-graphene and thymine-graphene have a very similar shape, like the thymine dimer created by UV light in DNA [5]. The thymine nucleobase is a pyrimidine derivative, which has a six-membered aromatic ring similar to a central structure of the benzene molecule, but with two nitrogen atoms in the ring instead of carbons. The resemblance of the central structural elements in these aromatic molecules allows suggesting that the formation and reverse dissociation of dimers is determined by analogous vibronic mechanisms. Thus, UV radiation of aromatic molecules, physisorbed on graphene, may lead to the appearance of covalent functionalization of graphene basal plane.

The purpose of this work is to apply developed in Refs. [1-3] the vibronic interactions calculation method for investigation of excited states of molecular dimers in DNA and molecules on graphene. In this work, the results of numerical calculations of the potential surface of bi-benzene (with a view to determining a pathway of formation of the thymine dimers in DNA) and the covalently bound structure of thymine molecule and graphene sheet (with a view to promoting the functionalization of graphene) are presented. The Raman spectra to determine how covalently bound structures differ from the initial ones were calculated using DFT (Density Function Theory) method. The calculated spectra are in a good agreement with available experimental data and are significantly different, depending on the presence or absence of covalent bonds between the compounds studied.

- [1] V. Krasnenko, V. Boltrushko, V. Hizhnyakov, "Vibronic interactions proceeding from combined analytical and numerical considerations: Covalent functionalization of graphene by benzene, distortions, electronic transitions", *J. Chem. Phys.* **144**(13), 134708 (2016). doi:10.1063/1.4944990
- [2] V. Boltrushko, V. Krasnenko, V. Hizhnyakov, "Pseudo Jahn-Teller effect in stacked benzene molecules", *Chem.Phys.* **460**, 90-96 (2015). doi:10.1016/j.chemphys.2015.03.006
- [3] V. Krasnenko, V. Boltrushko, V. Hizhnyakov, "Distorted allotropes of bi-benzene: vibronic interactions and electronic excitations. *IOP Conf.Ser.:J.Phys.:Conf.Ser.* **833**, 12009 (2017). doi:10.1088/1742-6596/833/1/012009.
- [4] V. Krasnenko, J. Kikas, M. G. Brik, "Modification of the structural and electronic properties of graphene by the benzene molecule adsorption", *Phys.B: Condens.Matter.* **407**(23), 4557-4561 (2012).
- [5] H. E. Johns, S. A. Rapaport, M. Delbrück, "Photochemistry of thymine dimers", *J Mol Biol.* **4**, 104-114, (1962). doi:10.1038/197484a0
- [6] W. J. Schreier, T. E. Schrader, F. O. Koller, et al. "Thymine dimerization in DNA is an ultrafast photoreaction", *Science.* **315**(5812), 625-629 (2007). doi:10.1126/science.1135428.
- [7] J. A. Marteiijn, H. Lans, W. Vermeulen, J. H. J. Hoeijmakers, "Understanding nucleotide excision repair and its roles in cancer and ageing". *Nat.Rev.Mol.Cell Biol.* **15**(7), 465-481 (2014). doi:10.1038/nrm3822.

*Corresponding author: Veera.Krasnenko@ut.ee

Dynamics of paired electrons and holes in bilayer nonlinear lattices and transport of the pairs by soliton-like excitations

Alexander P. Chetverikov^{*1}, Werner Ebeling², Eckehard Scholl³, and Manuel G. Velarde⁴

¹*Saratov National Research State University, Astrakhanskaya, 83, 410012, Saratov, Russia*

²*Humboldt-University Berlin, Newtonstrasse, 15, 12489, Berlin, Germany*

³*Technische Universität Berlin, Hardenbergstrasse, 36, 10623, Berlin, Germany*

⁴*Universidad Complutense Madrid, Paseo Juan XXIII, 1, 28040, Madrid, Spain*

Crystal-lattice bilayers with an-harmonic Morse interactions doped with electrons in one layer and with holes in the other [1] are considered. Computer numerical simulations permit to follow the evolution consequence of the coupling of the dynamics of an electron and a hole to lattice soliton-like excitations propagating along crystallographic axes of one or both of the an-harmonic bi-layer structure.

First we study the dynamic changes of super-sonic solitons, or crowdions, created in one or both layers and running along closely packed atomic rows in each crystal lattice layer [2]. Then we study the behavior of single electrons and holes in the polarization field induced by the lattice soliton deformations in the frame of the tight-binding model.

Finally, we investigate the effect of Coulomb attraction between electrons and holes, eventually leading to the formation of electron-hole pairs and we discuss applications such as the control of the dynamics of electron-hole pairs by soliton-like excitations in a form of electron-hole pair surfing [3].

This work was supported by the grant 16-12-10175 from the Russian Scientific Foundation.

- [1] K. Lee, J. Xue, D. C. Dillen, K. Watanabe, T. Taniguchi, E. Tutuc, Giant Frictional Drag in Double Bilayer Graphene Heterostructures, *Phys. Rev. Lett.* **117** (2016) 046803
- [2] A. P.Chetverikov, W. Ebeling, M. G.Velarde, Localized nonlinear, soliton-like waves in two-dimensional an-harmonic lattices, *Wave Motion* **48**(2011) 753
- [3] A. P.Chetverikov, W. Ebeling, M. G. Velarde, Soliton assisted control of source-to-drain electron transport along natural channels -crystallographic axes- in two-dimensional triangular crystal lattices. *Eur. Phys. J. B* **89** (2016) 196

*Corresponding author: chetvap@rambler.ru

Flux-flow spin Hall effect in type-II superconductors

A. Vargunin*^{1,2} and M.A. Silaev¹

¹*Department of Physics and Nanoscience Center, University of Jyväskylä, Jyväskylä, FI-40014, Finland*

²*Institute of Physics, University of Tartu, Tartu, EE-50411, Estonia*

We predict the very large spin Hall effect in type-II superconductors which mechanism is drastically different from the previously known systems. We find that in the flux-flow regime the spin is transported by the spin-polarized Abrikosov vortices moving under the action of the Lorenz force in the direction perpendicular to the applied electric current. Due to the large vortex velocities the spin Hall angle can be of the order of unity in realistic systems based on the high-field superconductors or the recently developed superconductor/ferromagnetic insulator proximity structures. We suggest the high-frequency generator of the pure spin currents stemming from the periodic structure of moving vortex lattices and discuss the inverse flux-flow spin Hall effect when the injected spin current generates longitudinal driving force on vortices and the transverse voltage in result of their motion.

[1] A. Vargunin, M.A. Silaev, arXiv:1803.03442.

*Corresponding author: artjom.vargunin@gmail.com

Nonlinear atomic vibrations and structural phase transitions in strained carbon chains

George Chechin^{*1}, Dmitry Sizintsev¹, and Oleg Usoltsev¹

¹*Institute of Physics, Southern Federal University, Stachki ave. 194, Rostov-on-Don, 344090, Russia*

Monoatomic carbon chains can exist in two different modifications. The first one is polyynes, representing the chain with alternating single and triple bonds [chemical structure $(-C\equiv C-)_n$]. The second modification is cumulene, representing the chain with double bonds [chemical structure $(=C=C=)_n$]. Because of many unique mechanical, physical, and chemical properties, carbyne is considered as perspective material for various nanodevices, for hydrogen storage, etc.

We study the properties of strained carbon chains in [1, 2] with the aid of *ab initio* simulation based on the Density Functional Theory (DFT). During this investigation, we revealed an unexpected phenomenon of softening of the longitudinal π -mode vibrations above a certain critical value of the strain. We found that for strains lower than $\eta = 11\%$ cumulene demonstrates monotonic hard type of nonlinearity (the frequency grows with increase of the π -mode amplitude a). However, for $\eta > 11\%$ there is a certain range of amplitudes a in which soft nonlinearity occurs, namely, the frequency of the π -mode abruptly decreases and then again begins to increase.

The phenomenon of vibrational modes softening is well known in the theory of structural phase transitions where by condensation ("freezing") of such modes one tries to explain the nature of the displacement-type phase transitions. This is the so-called concept of soft modes. In the majority of the papers on this subject, soft modes are treated in purely phenomenological manner with some vague arguments about the change of electron-phonon interactions in crystal under change of such external parameters as temperature and pressure. In contrast, in our study a soft vibrational mode in cumulene appears as a direct result of the *ab initio* simulation without any additional assumptions.

We explain the phenomenon of the π -mode softening, above the critical value of the strain, by the fact that the old atomic equilibrium positions become unstable and two new equilibrium positions appear near each of them. Vibrations in the vicinity of these new equilibrium positions correspond to the softening of the π -mode. In turn, condensation of the π -mode leads to a new atomic equilibrium configuration that corresponds to the Peierls phase transition. After this transition, the unit cell turns out to be twice as large as that of cumulene, and the carbon chain transforms into another carbyne form, polyynes, with bond lengths alternation.

In [2] and in the present report, we discuss not only the condensation of the π -mode, but also condensation of two other symmetry-determined nonlinear normal modes, which are possible in cumulene chains. With the aid of DFT and molecular dynamics simulations combined with some group-theoretical methods [3], we predict the possibility of existence of two new types of carbon chains, besides cumulene and polyynes. They both possess alternation of bond lengths, but with different alternating schemes compared to that of the polyynes.

The Peierls phase transition in cumulene under certain strain was revealed previously in [4]. This transition leads to the radical change of carbyne electron spectrum. As a result, an energy gap in the electron spectrum appears and the conductive cumulene transforms into polyynes which is semiconductor or insulator. Note, that the paper [4] actually deals with the static structure of strained carbyne. In contrast, the problem of strong nonlinear atomic vibrations in strained carbon chains was studied for the first time in our paper [1].

It seems that the obtained results may be used in construction of new nanotechnology devices, where electrical properties of carbyne can be controlled by mechanical strain. The presented results can also be useful for searching new forms of carbyne, which are predicted in this work.

[1] G. Chechin, D. Sizintsev, O. Usoltsev, *Letters on Materials* **6**, 146 (2016).

[2] G. Chechin, D. Sizintsev, O. Usoltsev, *Computational Material Science* **138**, 353 (2017).

[3] G. Chechin, D. Ryabov, K. Zhukov, *Physica D* **203**, 121 (2005).

[4] V. Artyukhov, M. Liu, B. Yakobson, *Nano Lett.* **14**, 4224 (2014).

*Corresponding author: gchechin@gmail.com

Spin-1/2 Heisenberg model on one-third-depleted square lattice: exact diagonalization study

P. Rubin*¹

¹*Institute of Physics, University of Tartu, Ostwaldi 1,50411, Tartu, Estonia*

In charge ordered layered nickelate $\text{La}_4\text{Ni}_3\text{O}_8$ the Ni ions in NiO_2 planes are separated into charge ordered Ni^{1+} (spin 1/2) and Ni^{2+} (spin 0), so that spin-1/2 stripes are formed at 45 degrees relative to the Ni – O bonds [1,2]. The Ni^{1+} ions form an AF arrangement in analogy with the CuO_2 planes of the cuprate superconductors. Magnetic properties of these NiO_2 planes can be described in the framework of the Heisenberg model on one-third-depleted square lattice, where sites with zero spin are removed from the square lattice (one-third part of the number of sites). This model takes into account the antiferromagnetic nearest- and next-nearest exchange interactions (J_1 and J_2).

We investigated this model with the use of the exact diagonalization with account of periodic boundary conditions. Small lattices with $N = 16$ and $N = 24$ were considered. The energies of the ground state, low-lying states and spin-spin correlation functions were obtained with the use of SPINPACK code (the Lanczos exact diagonalization) in the entire range the parameter $0 < p < 1$, where $p = J_2/(J_1 + J_2)$. It was found that the dependencies of the spin-spin correlation functions on p have the inflection point at $p \approx 0.66$. This value correlates with $p_c \approx 0.64$ obtained by the stochastic series expansion quantum Monte Carlo method wherein AFLRO disappears [2] and the lattice breaks up into dimers.

- [1] J. Zhang, Y.-S. Chen, D. Phelan, H. Zheng, M. R. Norman, and J. F. Mitchell, “Stacked charge stripes in the quasi-2D trilayer nickelate $\text{La}_4\text{Ni}_3\text{O}_8$ ”, *PNAS* **113**, 8945 (2016).
- [2] H.-M. Guo, T. Mendes-Santos, W. E. Pickett, and R. T. Scalettar, “Magnetic order-disorder transitions on a one-third-depleted square lattice”, *Phys.Rev. B* **95**, 045131 (2017).

*Corresponding author: rubin@ut.ee

Dynamical Jahn-Teller effect: time evolution of vibronic states in conical intersection

V. Hizhnyakov^{*1}, H. Kaasik¹, and K. Pae¹

¹*Institute of Physics, University of Tartu, W. Ostwaldi Str 1, 50411, Tartu, Estonia*

An essential feature of vibronic systems with electronic degeneracy is the existence of the conical intersections in the adiabatic potential surfaces. The behavior of a system near a conical intersection is governed by strong non-adiabaticity causing fast transitions between the crossing branches of the APES. This results in appearance of the resonant states. In $E \times e$ Jahn-Teller systems, these states are known as Slonczewski resonances. One expects that the characteristic time of formation of Slonczewski states is short, 10-100 fs. A specific aspect of the dynamics of the $E \times e$ Jahn-Teller systems in the vicinity of the conical intersection is the participation of the rotation around the centrum. This rotation participates in Slonczewski resonance states.

We have developed theory of Slonczewski states. Wave functions of these states can be taken in the form $X^{(l)}(r, \varphi) = r^{-1/2} e^{il\varphi} \chi^{(l)}(r) |\phi_{e,\varphi}\rangle$, where l is integer rotational quantum number, $|\phi_{e,\varphi}\rangle$ is the electronic function in adiabatic approximation, $\chi^{(l)}(r)$ is the radial vibrational function. It satisfies the following equation

$$(-d^2/d\xi^2 + \xi - \varepsilon_m + (4l^2 + 1)/16\xi^2) \chi^{(l)}(\xi) = 0$$

where r and φ are polar coordinates of the vibrational mode, $\xi = (2k)^{1/3} r$, ε_m is the energy of the state. For small l one can neglect also the last term in the brackets. Then $\chi_m^{(l)}(\xi) \approx Ai(\xi - \varepsilon_m)$ are the Airy functions.

Slonczewski states are not the stationary ones; they are the wave-packets of the stationary vibronic states of the $E \times e$ problem. Knowledge of $X^{(l)}(r, \varphi)$ allows us to find the time evolution $L_m^{(l)}(t)$ of them using the Fock-Krylov theorem. We have derived the following equation for the Fock-Krylov function:

$$L_m^{(l)}(t) = \sum_k \left(\left| D_{k;m}^{(l)} \right|^2 \exp(itE_k^{(l+1/2)}) + \left| D_{k;m}^{(l-1)} \right|^2 \exp(itE_k^{(l-1/2)}) \right).$$

Here $E_k^{(j)}$ are the energies of the stationary vibronic states,

$$D_{k;m}^{(l)} = \frac{1}{2} \sum_n \left(C_{2n,k}^{(l+1/2)} S_{n,m}^{(l,l)} + iC_{2n+1,k}^{(l+1/2)} S_{n,m}^{(l+1,l)} \right),$$

$S_{n,m}^{(l,l)}$ are the eigenvectors of Slonczewski states in harmonic basis, $C_{n,k}^{(j)}$ are the eigenvectors of the vibronic Hamiltonian.

Presented equation describes only phase relaxation of femtosecond scale of the Slonczewski state in conical intersection. The energy loss of these states takes place as the emission of phonons; its characteristic time is 1 - 10 ps. This energy loss has been studied in detail in [1]. To take this loss into account one needs to add to the energies $E_k^{(j)}$ the imaginary summands $i\gamma_k^{(j)}$ caused by the interaction with phonons. Here we use $\gamma_k^{(j)}$ calculated in [1,2]. Numerical calculations of the Fock-Krylov functions are in progress.

[1] K. Pae, and V. Hizhnyakov, *J Chem. Phys.* **147**, 084107 (2017)

[2] K. Pae and V. Hizhnyakov, *J. Chem. Phys.* **145**, 64108 (2016)

*Corresponding author: hizh@ut.ee

Substitution effects in FeAs₂: A route to advanced materials

A. Pishtshev*¹ and P. Rubin¹

¹*Institute of Physics, University of Tartu, W. Ostwaldi 1, 50411 Tartu, Estonia*

By using density functional theory we studied how the substitution effects may change the structural and electronic subsystems of the binary iron pnictide FeAs₂ [1]. The Ni and Mg substitutions were considered. The main results of our research are the following:

(I) Both substitutions lead to isolator-metal transition at a moderate impurity concentration. However, the structural effects of the stoichiometric replacements, Fe → Ni and Fe → Mg, are cardinally different. Unlike the Ni-doping, the Mg dopant incorporated into the iron site has a most pronounced influence on the lattice: by occupying a non-central position in the unit cell it features the local lattice distortion.

(II) The structural instability is caused by the local pseudo Jahn-Teller effect (pJTE). Due to the enhanced vibronic interaction in the Mg-[FeAs₆] cluster, the pJTE promotes the on-site symmetry breaking.

(III) Significantly, such off-center displacement of the pJTE origin associated with a partial replacement of Fe by Mg is firmly retained in the impurity configuration. This implies [1] that by controlling the range of Fe → Mg replacements one can explore the potential of large vibronic couplings with respect to the possible superconducting function of the material.

[1] A. Pishtshev, P. Rubin, "Enhanced vibronic interaction caused by local lattice symmetry lowering in the (Fe, Mg)As₂ ternary system", *Journal of Applied Physics* **123** (16), 161557 (2018).

*Corresponding author: aleksandr.pishtshev@ut.ee

Predictive modeling with TensorFlow

D.Nevedrov*¹

¹*T. Rowe Price, Colorado Springs, CO, USA*

TensorFlow is an open source software library for numerical computations and is great tool that is used to drive advancements in machine learning. The software uses flow graphs where nodes represent mathematical operation, and the graph edges represent multidimensional data arrays, or tensors that are exchanged between nodes. *TensorFlow* was originally developed for conducting deep neural network research but it is also applicable to a variety of other domains. Combination of increasing processing power and data storage capabilities, plus the scalability and portability lead to a number of useful business and science application of *TensorFlow*. One of the practical uses of *TensorFlow* is the predictive and linear modeling, which can help model the behavior based on the provided set of data. The data is packaged as a model, then this model is used to predict other, future values that are not part of the set. Specifically we obtain the data for a number of financial markets, and use *TensorFlow* to build, train, perform a data analysis and predict the trend on the market.

*Corresponding author: dmitri_nevedrov@hotmail.com

Time dependent (transient) theory of resonant secondary emission at two-step absorption of two light pulses

I. Rebane*¹

¹*Institute of Physics, University of Tartu, Ravila 14c, Tartu 50411, Estonia*

The time dependent (transient) theory of resonant secondary emission (light scattering and luminescence) at two step-absorption of two different light pulses with arbitrary duration in the electronic four-level model ($0 \rightarrow 1 \rightarrow 2 \rightarrow 0'$) is proposed. The third step of the time dependent perturbation theory is applied. The transient spectrum $I(\Omega, t)$ is defined as the photon counting rate at the instant of time t when the spectral instrument with spectral resolution η is tuned to the frequency Ω . In general case three lines exist: the resonant scattering line ($0 \rightarrow 0'$) (Fig.1 A, Fig.2 at $z = 35$), the luminescence line ($2 \rightarrow 0'$) (Fig.1 B and C, Fig.2 at $z = 0$), and the third line which describes process in which after absorption of the first pulse ($0 \rightarrow 1$) which takes system to the first excited level 1, the scattering of the second pulse ($1 \rightarrow 0'$) takes place (Fig.1 D, Fig.2 at $z = 20$).

This work was supported by Estonian Ministry of Education and Research through the Institutional Research Funding IUT2-27 "Nonlinear theory of solids and fundamental fields".

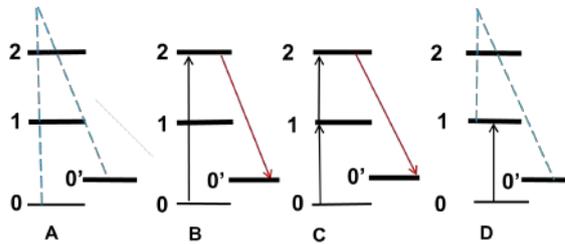


Figure 1: Scheme of the interposition of the four levels and the possible transitions between them.

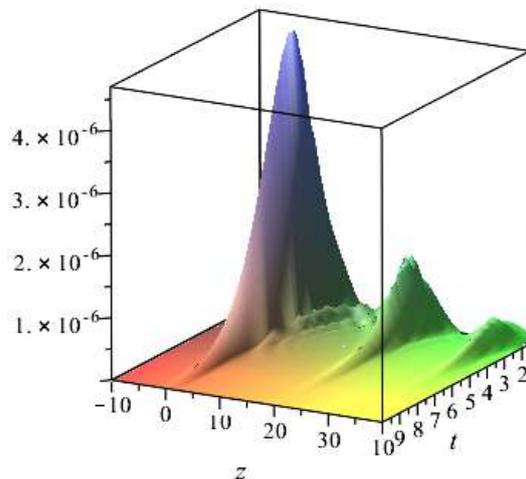


Figure 2: The transient spectrum $I(\Omega, t)$ at $\omega_1 - \Omega_{01} = -15\gamma_2$, $\omega_2 - \Omega_{12} = -20\gamma_2$, $\Delta_1 = \Delta_2 = \gamma_1 = \gamma_2$, $\gamma_{0'} = 0$, $T = \gamma_2^{-1}$, $\eta = \gamma_2$. Here ω_1 and ω_2 are the frequencies of the maxima of the pulses; Ω_{01} , Ω_{12} and Ω_{20} are the transition frequencies; γ_1 , γ_2 and $\gamma_{0'}$ are the rates of energy relaxation; Δ_1 and Δ_2 are the spectral widths of the pulses; T denotes the time between pulses. Variable $z \equiv \Omega - \Omega_{20'}$ is given in units of γ_2 , and variable t is given in units of γ_2^{-1} . $I(\Omega, t)$ is given in arbitrary units.

*Corresponding author: inna.rebane@ut.ee

Tunneling in resonance Raman scattering

V. Hizhnyakov^{*1}, K. Kugel², and I. Tehver¹

¹*Institute of Physics, University of Tartu, Ostwaldi 1,50411, Tartu, Estonia*

²*Institute for Theoretical and Applied Electrodynamics, Russian Academy of Sciences, Izhorskaya Str. 13, Moscow 125412, Russia*

The Raman scattering (RRS) by a system performing tunneling motion in the ground state is considered. We suppose that the potential energy of the ground state has two minima resulting in the existence of the tunneling states with different energies. The excited states, dominantly contributing to the Raman polarization have a single minima for the coordinate associated with the tunneling motion. Correspondingly, the Raman active vibrations have different equilibrium positions in the different minima of the potential surface of the tunneling system. To describe RRS we use the time-domain approach (see e.g. [1]), having close analogy to the developed by Lax [2] time-domain approach for the Fourier transform of absorption. We have found that the first-order Raman scattering of a vibration interacting with the tunneling system takes place only if it is accompanied by the tunneling transition, i.e. only transitions

$$\begin{aligned} |\{n\}\rangle_+ \rightarrow |1_j\rangle_- &= \frac{1}{\sqrt{2}} (|\{n\} \pm 1_j\rangle_1 - |\{n\} \pm 1_j\rangle_2) \\ |\{n\}\rangle_- \rightarrow |1_j\rangle_+ &= \frac{1}{\sqrt{2}} (|\{n\} \pm 1_j\rangle_1 + |\{n\} \pm 1_j\rangle_2) \end{aligned}$$

should be considered, where $|\{n\}\rangle_{\pm}$ and $|\{n\} \pm 1_j\rangle_{\pm}$ denote the initial and final vibrational states (subscripts \pm mark even (+) or odd (-) tunneling states), $\pm 1_j$ denotes the created or destroyed vibrational quantum, subscripts 1 and 2 indicate the first and second minima of potential surface, between which the tunneling transitions take place. Thus, only the Raman scattering together with the transitions from even to odd and from odd to even tunneling states takes place with remarkable amplitudes. Consequently, in the Raman scattering of a tunneling system instead of the Raman line with frequency ω_j one will observe the doublet line with frequencies $\omega_j \pm \bar{\epsilon}(1 - 4\xi_j^2)$, where “+” corresponds to the lower initial tunneling state and “-“ to the upper initial tunneling state. Thus, the Raman lines of tunneling systems split to two components; the splitting frequency is

$$\delta\omega_j = 2\bar{\epsilon}(1 - 4\xi_j^2),$$

where $\bar{\epsilon}$ is the tunneling splitting, $\xi_j = \sqrt{\omega_j/2\hbar}x_{0j}$ denotes the constant of vibronic interaction with phonon j , x_{0j} is the change of the equilibrium position of phonon j at the electronic transition.

Describing RRS in a time-domain in full analogy with the Fourier transform of absorption $F(t)$ [2], we find the following equations for the Fourier amplitudes of the first-order Raman scattering between odd (even) and even (odd) tunneling states

$$A_{1_j}^{(-+)}(t) \propto \langle 1_{\pm j} | e^{iH_e} e^{-iH_g} | 0_{\mp} \rangle = \xi_j (e^{i\omega_j t} - 1) F(t).$$

Finally, we note that analogous splitting of Raman lines in tunneling system will be observed for all odd-order Raman scattering lines. However, the even-order Raman lines are not split.

- [1] V. Hizhnyakov, I. Tehver, “Resonance Raman Scattering of Multimode Systems: Fourier Amplitude Approach”, *J. Raman Spectroscopy*, **24**, 653-660 (1993).
 [2] M. Lax, “The Franck-Condon Principle and Its Application to Crystals”, *J. Chem. Phys.* **10**, 1752-1760 (1952).

*Corresponding author: vladimir.hiznjakov@ut.ee

Spontaneous parametric-down conversion in plasmonic structures

A. Loot*¹ and V. Hizhnyakov¹

¹*Institute of Physics, University of Tartu, Ostwaldi 1,50411, Tartu, Estonia*

Spontaneous parametric down-conversion (SPDC) is one of the main processes for the generation of entangled photon pairs. However, SPDC in a bulk crystal is very weak, the yield is only around 10^{-12} , and for the efficient generation, at least a millimeter long crystal is required. Several attempts have been made in order to increase the efficiency of SPDC and to miniaturize the source. In this work, we explore the idea to use resonant surface waves in order to enhance SPDC and to open ways to miniaturize the source of entangled photon pairs [1,3].

To model the SPDC in resonant structures we used transfer-matrix method extended for second-order nonlinear processes [2]. The SPDC is considered as a quantum analog of difference-frequency generation. Also, the infinite plane waves were replaced with realistic beams (e.g. Gaussian beam) by another extension [3]. All the code developed is available at GitHub (github.com/ardiloot/NonlinearTMM).

We studied the enhancement of SPDC in three types of resonant modes: ordinary surface plasmon polaritons (SPPs), long-range SPPs (LRSPPs) and guided dielectric waves (GDWs). In the case of SPPs, the enhancement factor of SPDC is up to 10^4 . This enhancement is only beneficial in the case of miniature sources up to $64\ \mu\text{m}$ due to the limitation of coherent buildup distance. LRSPPs and GDWs extend the coherent build-up distance considerably (up to several millimeters), however new limiting factor arises: as the resonances of LRSPPs and GDWs are very narrow, the enhancement factor is limited by the weak interaction with a usual Gaussian beam.

- [1] A. Loot, I. Sildos, and V. Hizhnyakov, "Enhanced spontaneous parametric down-conversion in a metal-dielectric interface," *IEEE Xplore*, 7342484, pp. 451-453 (2015).
- [2] A. Loot and V. Hizhnyakov, "Extension of standard transfer-matrix method for three-wave mixing for plasmonic structures," *Applied Physics A*, 123:152(3), pp. 1-7 (2017).
- [3] A. Loot and V. Hizhnyakov, "Modeling of enhanced spontaneous parametric down-conversion in plasmonic and dielectric structures with realistic waves," *Journal of Optics*, in-press (2018)

*Corresponding author: ardi.loot@ut.ee

Magnetic and Structural Properties of the Trirutile-type 1D Heisenberg Antiferromagnet CuTa₂O₆

A. Golubev^{*1}, R.E. Dinnebier¹, A. Schulz¹, R.K. Kremer^{†1}, H. Langbein²,
A. Senyshyn³, J.M. Law⁴, T. Hansen⁵, H.-J. Koo⁶, and M.-H. Whangbo⁷

¹Max Planck Institute for Solid State Research, Stuttgart, Germany

²Institut für Anorganische Chemie der Technischen Universität Dresden, Dresden, Germany

³Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany

⁴Dresden High Magnetic Field Laboratory (HLD), Dresden, Germany

⁵Institut Laue-Langevin, Grenoble, France

⁶Kyung Hee University, Seoul, Republic of Korea

⁷North Carolina State University, North Carolina, USA

CuTa₂O₆ crystallizes with a monoclinically distorted trirutile structure type [1,2]. By detailed high temperature neutron and x-ray powder diffraction measurements we mapped the structural phase transition to the tetragonal trirutile structure-type at 500K. The structural phase transition was ascertained by Raman scattering experiments. *Ab initio* GGA+U density functional calculations of the spin exchange parameters, magnetic susceptibility and isothermal magnetization measurements constitute CuTa₂O₆ as one-dimensional Heisenberg quantum antiferromagnet with predominant nearest-neighbor spin exchange interaction $J_{nn} \sim 50$ K. Long-range magnetic order was not detected down to 0.4 K.

- [1] I. Krabbes, H. Langbein, "Herstellung von CuTa₂O₆ - von der Trirutil - zur Perowskit- Struktur", Z. Naturforsch. **51**(b), 1605-1610 (1996).
- [2] H. Langbein, M. Bremer, I. Krabbes, "CuX₂O₆ and Ba₃CuX₂O₉ (X = Nb, Ta): Influence of the preparation conditions on phase formation and phase composition", *Solid State Ionics* **101**, 579-584 (1997).

*Corresponding author: a.golubev@fkf.mpg.de

†Corresponding author: rekre@fkf.mpg.de

Supersonic solitons in Fermi-Pasta-Ulam chain

V. Hizhnyakov*¹

¹*Institute of Physics, University of Tartu, W. Ostwaldi Str 1, 50411, Tartu, Estonia*

The simplest model of anharmonic atomic lattices is the known Fermi-Pasta-Ulam (FPU) chain [1], consisting of identical atoms. FPU used the following equations of motion of atomic displacements:

$$\ddot{u}_n = k(u_{n+1} + u_{n-1} - 2u_n) [1 + \lambda(u_{n+1} - u_{n-1})],$$

where $n = 0, 1, \dots, N-1$, u_n is displacement of atom n , $k = k_2/m$, $\lambda = k_3/k_2m$, k_2 is the elastic spring, k_3 is the constant of cubic anharmonicity, m is the mass of an atom. FPU have found that for $\lambda \neq 0$ the initially displaced atom first performs decaying vibrations; but then after a while the initial state is restored. This means that the system does not exhibit thermalization - a fully unexpected result.

It is believed that there are no solitons in the FPU chain, but they do exist in the generalized FPU chain, having the additional term $\mu ((u_{n+1} - u_{n-1})^2 + (u_n - u_{n-1})(u_n - u_{n+1}))$ in the equation of motion (μ is parameter of quartic anharmonicity). However, we found [2] that in FPU chain there may exist solitons, although exotic ones - supersonic.

We have found the following solutions of the equations of motion of the generalized FPU chain, describing the envelopes of the displacements $\chi_n = u_n - u_{n+1}$ and $\psi_n = u_n + u_{n+1}$ [2]:

$$\chi = \sqrt{\frac{2}{3\mu - 4\lambda^2/(1-v^2)}} \frac{\varepsilon' \cos(\omega'(t+vx))}{\cosh(\varepsilon'(x-vt))}, \quad \psi = \frac{2\lambda\varepsilon'}{3\mu(1-v^2) - 4\lambda^2} \tanh(\varepsilon'(x-vt)),$$

where $\omega' = \omega(1+v^2)^{-1/2}$ and $\varepsilon' = \omega(\omega^2 - \omega_M^2)^{1/2}(1+v^2)^{-1/2}$, x is coordinate, t is time, v is velocity of soliton.

There are two types soliton solutions: a) the well-known solitons with subsonic velocity $v < 1$ (they exist, if $|v| < (1 - 4\lambda^2/3\mu)^{1/2}$, i.e. if the cubic anharmonicity is small), b) solitons with supersonic velocity $v > 1$. Such solitons may exist for chains with any cubic anharmonicity λ , supposing that $\mu < 4\lambda^2/3(1-v^2)$. They exist also in Fermi-Pasta-Ulam chain (having $\mu = 0$).

As far as we know, supersonic solitons in FPU chain have not yet been observed. For these solitons, the cubic anharmonicity plays a decisive role: the moving mode is stabilized by the moving deformation of the lattice caused by this anharmonicity.

- [1] E. Fermi, E.J. Pasta, S. Ulam, (1955). "Studies of Nonlinear Problems" (PDF). Document LA-1940. Los Alamos National Laboratory.
 [2] V. Hizhnyakov, Supersonic motion of high frequency vibrational soliton in monatomic chain, arXiv:17.09.06008.

*Corresponding author: vladimir.hiznjakov@ut.ee

Origin of ground state of $E \otimes e$ Jahn-Teller system

Kaja Pae*¹ and V. Hizhnyakov¹

¹*Institute of Physics, University of Tartu, W. Ostwaldi Str 1, 50411, Tartu, Estonia*

The symmetry of the ground state in the Jahn-Teller systems is a subject of long discussion. Allowance for linear and quadratic vibronic couplings in these systems leads to the appearance of three equivalent minima on the adiabatic potential energy surface (APES). The system can perform tunneling between these minima. Symmetry considerations show that of the three lowest states, here one in singlet and belongs to the representation A_1 , and the two remaining states form a doublet belonging to E-representation. The question here is, which state has a lower energy. At first, Bersuker (1961) came to the conclusion that in the case of deep minima of APES the ground state is nondegenerate. Somewhat later O'Brien (1964), who considered tunneling as a hindered rotation, came to the conclusion that state E has a lower energy than state A_1 . This conclusion was supported by Ham (1968), who showed that in the adiabatic approximation such an order of lower levels follows from the presence of the geometric Berry phase. After the work of O'Brien and Ham, it became widely accepted that the symmetry of the ground state of the vibronic system coincides with the symmetry of the initial electronic state.

However, this belief was shattered after the findings of Moate et. al and Manini et al in 1996 year that for some parameter values the ground state in the Jahn-Teller $H \otimes h$ problem is nondegenerate. A further study of several authors led to the conclusion that in the adiabatic approximation the ground state is degenerate if the dominant motion occurs around an odd number of conical intersections of APES, and this is not so if this number is even. However, the question of the origin of the ground state in systems with strong nonadiabaticity remained unanswered.

We carried out a study of the vibronic states of $E \otimes e$ Jahn-Teller systems with numerically exact allowance for nonadiabaticity for various values of linear (k_1) and quadratic (k_2) vibronic couplings, which enabled us to answer this long-standing question. A remarkable property of $E \otimes e$ Jahn-Teller systems is the difference of the origin of its states in two limiting cases: 1) $k_2 = 0$ and 2) $k_1 = 0$, both with axial symmetry of APES. In the first case the rotational momenta are half-integer, while in the second case they are integer. As a result, in the first case the ground state is doublet, and in the second case it is singlet for any values of k_1 or k_2 . However if both, k_1 and k_2 differ from zero, then the order of the lower states should be found numerically. We have developed an algorithm that allows such calculations [1]. It follows from these calculations that if the quadratic interaction is weak ($|k_2| \ll 1$), then the ground state is doubly degenerate regardless of the strength of the linear interaction. However, in the opposite case of small $k_1 < 0.7$ and for $1 - k_2 < 0.07$ the order of the lowest levels is different.

Finally, we note that our theory allows us to take into account the phonon continuum. This can be done by applying the method of taking phonons into account in the Jahn-Teller systems, recently developed by us (see Ref. [2]). In addition, this theory can be directly generalized to account for the anharmonicity of vibrations. With such a generalization it will be possible, for example, to calculate that the vibronic states of the Renner-Teller systems which are strongly deformed due to a quadratic vibronic coupling.

[1] K. Pae, and V. Hizhnyakov, *J. Chem. Phys.* **147**, 084107 (2017).

[2] K. Pae and V. Hizhnyakov, *J. Chem. Phys.* **145**, 64108 (2016).

*Corresponding author: kaja.pae@ut.ee

Two orbital superconductor with anisotropic pairing: characteristic lengths

G. Litak^{*1,2}, T. Örd³, K. Rägo³, and A. Vargunin^{3,4}

¹Lublin University of Technology, Faculty of Mechanical Engineering, A Nadbystrzycka 36, PL-20618 Lublin, Poland

²AGH University of Science and Technology, Department of Process Control, Mickiewicza 30, PL-30-059 Krakow, Poland

³Institute of Physics, University of Tartu, W. Ostwaldi Str. 1, 50411 Tartu, Estonia

⁴Department of Theoretical Physics, The Royal Institute of Technology, Stockholm, SE-10691 Sweden

The two-orbital superconducting state is modeled by inter-site intra-orbital attractive Hubbard correlations together with inter-orbital pair-transfer interactions. The influence of bands filling on the temperature dependencies of the sizes of Cooper pairs with d -wave symmetry in different orbitals is analyzed. An interband proximity effect was also reported in analogy to the on site attractive negative U interaction case which was studied earlier [1].

- [1] G. Litak, T. Örd, K. Rägo, A. Vargunin, "Cooper pairs in a two-orbital superconductor: bands filling effect on pair sizes", *Journal of Physics: Conf. Series* **833** 012017 (2017).

*Corresponding author: g.litak@pollub.pl

On the temperature behavior of Cooper pairs sizes in a two-band superconductor

T. Örd*¹, K. Rågo¹, A. Vargunin^{1,2}, and G. Litak³

¹*Institute of Physics, University of Tartu, W. Ostwaldi Str. 1, 50411 Tartu, Estonia*

²*Department of Theoretical Physics, The Royal Institute of Technology, Stockholm, SE-10691 Sweden*

³*Lublin University of Technology, Faculty of Mechanical Engineering, Nadbystrzycka 36, PL-20618 Lublin, Poland*

We study [1] the temperature dependencies of the mean sizes of the Cooper pairs in a two-band BCS-type *s*-wave superconductivity model with coupling cut-off in the momentum space. It is found that, in contrast to single-band systems, the size of Cooper pairs in the weaker superconductivity band can significantly decrease with a temperature increase due to an interband proximity effect. The relevant spatial behavior of the wave functions of the Cooper pairs is analyzed. The results also indicate a possibility that the size of Cooper pairs in two-band systems may increase with an increase in temperature.

- [1] T. Örd, K. Rågo, A. Vargunin, G. Litak, "Strong temperature effect on the sizes of the Cooper pairs in a two-band superconductor", *Eur. Phys. J. B* **91** (2) <https://doi.org/10.1140/epjb/e2017-80477-8> (2018).

*Corresponding author: teet.ord@ut.ee

Anomalous temperature dependence of vibronic spectra in low-dimensional systems

V. Boltrushko*¹ and V. Hizhnyakov¹

¹*Institute of Physics, University of Tartu, W. Ostwaldi Str 1, 50411, Tartu, Estonia*

In this communication, we consider a theory of the optical spectra of impurity centers in solids. The standard theory is failing to describe the temperature-dependent zero-phonon lines (ZPL) and phonon sidebands (PSB) in some quantum systems including ones with reduced dimensionality and changed statistics. Therefore, we present the generalizations that may tie the theory with the experiment without discrepancy.

It was shown previously [1] that ZPL and PSB are sensitive to the phonon dynamics such as softening of atomic bonds. These processes occur in disordered systems, where there are dynamical instabilities, and also in some quantum liquids. However, in this work, we step forward and replace asymptotic behavior with strict numerically-solved integrals. Thus, we can calculate numerically the vibronic spectra for the low-dimensional quantum systems at any temperature. We also check how the obtained theoretical results are backed with experiments.

- [1] V. Hizhnyakov, "Zero-phonon lines of systems with different dimensions and unconventional vibronic interactions", *J. Phys.: Condens. Matter* **24**, 104011 (2012).

*Corresponding author: vadim.boltrushko@ut.ee

Supermobile small size solitons in a monatomic chain with odd anharmonicity

A. Shelkan^{*1}, M. Klopov², and V. Hizhnyakov¹

¹*Institute of Physics, University of Tartu, W. Ostwaldi Str 1, 50411, Tartu, Estonia*

²*Tallinn University of Technology, Ehitajate tee 5, 19086 Tallinn, Estonia*

It is known that solitons of large size in atomic chains are highly mobile. The reason is that for these solitons it is possible to neglect the lattice discreteness and to consider solitons in the limit of a continuous medium. In this limit, the equations of motion can be rewritten in a moving reference frame and still have self-localized solutions. The discreteness of the atomic lattice brings new phenomena, one of which is the appearance of the Peierls-Nabarro barrier, causing the braking of solitons [1]. The smaller the soliton, the stronger the effect. Therefore, to study this braking, it is expedient to investigate solitons of small size.

In monatomic chain with nearest neighbor intersite anharmonic forces non-moving solitons (intrinsic localized modes (ILMs)) can exist if even anharmonicities dominate; increasing of odd anharmonicities may cause disappearance of ILMs. Therefore one expects that odd anharmonicity may also influence their mobility. In order to investigate this dependence, we performed calculations of solitons in monatomic chain with more than 99% of energy being localized on five central atoms. Frequency of these solitons equals $2.28 \omega_M$, where ω_M is the top phonon frequency. In these calculations, we have used dimensionless units with $k_2 = k_4 = 1$ and different values of k_3 (here k_2 is the elasticity of the chain, k_3 and k_4 are the cubic and quartic anharmonicity constants).

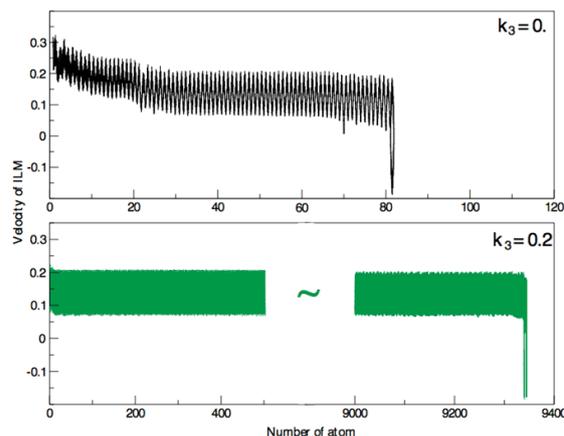


Figure 1: Dependence of the soliton velocity on its position.

increases.

Surprisingly, it was found that an increase of cubic anharmonicity leads to a large increase in mobility of solitons of a given size and frequency (see Fig.1); strong oscillations of velocity of soliton are due to Peierls-Nabarro barrier. Note very sharp soliton stop which occurs at the moment when the minimum velocity vanishes and soliton can no longer overcome the barrier.

Note also rather fast loss of velocities (and energy) in the final stage of motion. This indicates that the loss of energy by a soliton accelerates with time. A similar phenomenon, but for ILMs, was theoretically predicted in [2]. Finally we note the strong effect of the fifth anharmonicity on the Peierls-Nabarro barrier, which we observed: at a certain value of the parameter k_5 of this anharmonicity the barrier disappears and mobility of solitons strongly

[1] Yu. Kivshar, D. Campbell, *Phys. Rev. B* **48**, 3077-3081 (1993).

[2] V. Hizhnyakov, D. Nevedrov, A.J. Sievers, *Physica B* **316-317**, 132-135 (2002).

*Corresponding author: shell@ut.ee

Theory of superconducting surfaces and electrostatic doping dependence of critical temperature of high- T_c cuprate ultrathin films in the transverse electric field

P. Konsin*¹ and B. Sorkin¹

¹*Institute of Physics, University of Tartu, W. Ostwaldi Str 1, 50411, Tartu, Estonia*

In [1,2] an ultrathin high- T_c superconducting film being in contact with a normal metal from one side and a dielectric layer from another, the metal-insulator-superconductor structures and other interfaces between the film and dielectric substrate in the transverse electrostatic field are considered. A boundary condition for the Ginzburg-Landau wave function of a one-band superconductor at surfaces biased by a strong electrostatic induction is derived within the de Gennes approach. Detailed surface corrections to the bulk superconducting transition temperature T_c for the overdoped cuprate films in the positive and negative electric induction fields and for various film thicknesses are calculated. In the Thomas-Fermi approximation for two-dimensional electron gas the electrostatic doping parameter in superconducting films is derived. The dependences of the critical transition temperature T_c on the electrostatic doping in ultrathin cuprate-perovskite LSCO-type films in the whole region of their phase diagram are calculated using a phenomenological formula for T_c [3]. Recent experimental results for the electrostatic doping field effects in ultrathin superconducting films of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [4,5] are discussed. At this, some new results for electrostatically doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) ultrathin films are predicted.

- [1] P. Konsin, B. Sorkin, Electric field effects in high- T_c cuprates, *Phys.Rev. B* **58** (9), 5795-5802 (1998).
- [2] P. Konsin, B. Sorkin, Ferroelectric Polarization Effects in the Surface Superconductivity, *Ferroelectrics*. **436**, 1-4 (2012).
- [3] J L. Tallon, C Bernhard, H. Shaked, R L. Hitterman and J D. Jorgensen, Generic superconducting phase behavior in high- T_c cuprates: T_c variation with hole concentration in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$, *Phys. Rev. B*. **51** (18), 12911-12914 (1995).
- [4] A T. Bollinger, G. Dubuis, J. Yoon, D. Pavuna, J. Misewich and I. Božović, Superconductor-insulator transition in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ at the pair quantum resistance, *Nature* **472**, 458-460 (2011).
- [5] G. Dubuis, A T. Bollinger, D. Pavuna and I. Božović, Electric field effect on superconductivity in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, *J. Appl. Phys.* **111**, 112632-1-112632-6 (2012).

*Corresponding author: peet.konsin@ut.ee

Intrinsic localized modes in two atomic chains; reduction of cubic anharmonicity for gap modes

V. Hizhnyakov*¹

¹*Institute of Physics, University of Tartu, W. Ostwaldi Str 1, 50411, Tartu, Estonia*

It is already well-known fact that in monatomic anharmonic chains large-size self-localized vibrations (intrinsic localized modes (ILMs)) can exist being pushed up from the top of the phonon band to the forbidden area of frequencies by the anharmonicity [1]. However, in numerical studies these modes were found only for unrealistic pair potentials with dominating quartic anharmonicity. The reason was found to be the softening of the realistic pair potentials with increasing vibrational amplitude, caused by domination of cubic (odd) anharmonicity in these potentials. Due to these results, there was a conviction that ILMs in atomic chains with realistic pair-potentials can drop down from the optical band(s) to the gap(s) below (if there are such gaps), but they cannot split up from any phonon band.

We have developed an analytical theory of large size ILMs in two-atomic chain with cubic and quartic anharmonicity. In this theory, we came to another conclusion [2]: large-size ILMs in a two-atomic chain with realistic pair potentials cannot split up from the optical band. They also cannot split down from this band, but they can split up from the acoustic band, in opposite to conventional believe.

To understand the reasons of these unexpected results, let us consider the equations of motions of atoms in such a chain

$$M_0 \ddot{u}_{2n,t} = k_2(u_{2n-1} + u_{2n+1} - 2u_{2n}) \left(1 + \lambda(u_{2n+1} - u_{2n-1}) + \mu(u_{2n+1} - u_{2n-1})^2 + \mu(u_{2n} - u_{2n+1})(u_{2n} - u_{2n-1}) \right),$$

$$M_1 \ddot{u}_{2n+1,t} = k_2(u_{2n} + u_{2n+2} - 2u_{2n+1}) \left(1 + \lambda(u_{2n+2} - u_{2n}) + \mu(u_{2n+2} - u_{2n})^2 + \mu(u_{2n+1} - u_{2n+2})(u_{2n+1} - u_{2n}) \right).$$

Here u_n is the displacement of atom n , $\lambda = k_3/k_2$, $\mu = k_4/k_2$, k_2 is the elastic spring, k_3 and k_4 are the cubic and quartic anharmonicities, M_0 and $M_1 \leq M_0$ are masses of the atoms. One should take into account that vibrations with the frequencies close to the bottom of the optical band involve practically only light atoms; the heavy atoms then are almost at rest. Vibrations with the frequencies close to the top of the acoustic band involve practically only heavy atoms; the light atoms are almost at rest. Therefore, in the equation for the heavy atoms (with even number), the term with cubic anharmonicity parameter λ cancels; and only the quartic anharmonicity works, pushing the ILM from the acoustic band upward. At the same time, ILM cannot be split down from the optical band, if, as it is usually the case, the quartic anharmonicity is positive: $\mu > 0$. Only if quartic anharmonicity is negative ($\mu < 0$) they can split down from the optical band.

[1] A.M. Kosevich, A.S. Kovalev, *Zh. Eksp. Teor. Fiz.* **67**, 1793 (1974).

[2] V. Hizhnyakov, Intrinsic localized modes in two atomic chain; reduction of cubic anharmonicity for gap modes, arXiv: 1712.01110.

*Corresponding author: vladimir.hiznjakov@ut.ee

Index

- Örd, T., [49](#), [50](#)
- Archilla, J.F.R., [26](#)
Assani, M., [20](#)
- Barabanov, A.F., [12](#), [33](#)
Belemuk, A.M., [32](#)
Berger, H., [18](#)
Boltrushko, V., [51](#)
Busmann-Holder, A., [3](#)
- Caprara, S., [5](#)
Chechin, G.M., [21](#), [25](#), [38](#)
Chetverikov, A.P., [9](#), [36](#)
Chou, F.C., [17](#)
Chtchelkatchev, N.M., [12](#), [32](#)
Clemente-Juan, J.M., [2](#)
Colognesi, D., [20](#)
Coronado, E., [2](#)
- Dabrowski, J., [10](#)
Dinnebier, R.E., [46](#)
Dmitriev, S.V., [9](#), [21](#), [22](#)
Doi, Y., [26](#)
Dubinko, V., [28](#)
Dzebisashvili, D.M., [6](#), [33](#)
- Ebeling, W., [36](#)
Ekino, T., [24](#)
- Fedorov, S.V., [8](#)
- Gabovich, A.M., [24](#)
Gnezdilov, V., [17](#)
Golubev, A., [46](#)
Grilli, M., [5](#)
- Hansen, T., [46](#)
Heinmaa, I., [18](#)
Hizhnyakov, V., [40](#), [44](#), [45](#), [47](#), [48](#), [52](#), [54](#)
Hofmann, E., [10](#)
- Irwin, K., [28](#)
- Jaime, M., [18](#)
- Janowitz, C., [29](#)
Janson, O., [18](#)
- Kaasik, H., [40](#)
Karatsuba, E.A., [13](#)
Karazhanov, S., [34](#)
Kimura, M., [26](#)
Klesse, W.M., [10](#)
Klopov, M., [52](#)
Ko, J.-H., [3](#)
Komarov, K.K., [6](#)
Konsin, P., [53](#)
Koo, H.-J., [46](#)
Korovushkin, M.M., [33](#)
Korzniikova, E.A., [9](#), [21](#)
Kosevich, Yu.A., [27](#)
Kovaleva, N.N., [19](#)
Krasnenko, V., [35](#)
Kremer, R.K., [46](#)
Ksenofontov, V., [11](#)
Kugel, K.I., [4](#), [32](#), [44](#)
Kuz'min, V.I., [31](#)
- Langbein, H., [46](#)
Laptev, D., [28](#)
Law, J.M., [46](#)
Lemmens, P., [11](#), [17](#)
Lepri, S., [20](#)
Li, M.S., [24](#)
Litak, G., [49](#), [50](#)
Loot, A., [45](#)
- Mikheyenkov, A.V., [12](#), [32](#)
Moretti, P., [13](#)
Möller, A., [11](#)
- Nevedrov, D., [42](#)
Nikolaev, S.V., [31](#)
Noatschk, K., [10](#)
Nori, F., [4](#)
- Oleś, A.M., [16](#)
Ovchinnikov, S.G., [31](#)

Pae, K., 40, 48
Palii, A., 2
Piazza, F., 20
Pishtshev, A., 34, 41

Raimondi, R., 5
Rakhmanov, A.L., 4
Rebane, I., 43
Reuß, A., 11
Riviere, A., 20
Roleder, K., 3
Rosanov, N.N., 8
Rozhkov, A.V., 4
Rubin, P., 39, 41
Ryabov, D.S., 21, 25
Rägo, K., 49, 50
Röhler, J., 7

Saadatmand, D., 22
Sankar, R., 17
Sboychakov, A.O., 4
Schmeißer, D., 29
Scholl, E., 36
Schroeder, T., 10
Schulz, A., 46
Seibold, G., 5, 10
Senyshyn, A., 46
Sharafeev, A., 17
Shcherbinin, S.A., 21, 25
Shelkan, A., 52
Shepelev, I.A., 9
Sherman, A., 30
Sievers, A., 1
Silaev, M.A., 23, 37
Sizintsev, D., 38
Snamina, M., 16
Sorkin, B., 53
Stern, R., 18
Strugovshchikov, E., 34
Szymczak, H., 24

Tehver, I., 44
Terentyev, D., 28
Tsirlin, A.A., 15, 18
Tsukerblat, B., 2

Usoltsev, O., 38

Val'kov, V.V., 33
Valiulin, V.E., 12
Vargunin, A., 37, 49, 50
Velarde, M.G., 36

Veretenov, N.A., 8
Voitenko, A.I., 24

Weickert, F., 18
Whangbo, M.-H., 46
Wulferding, D., 11

Xiong, D., 22

Zolotaryuk, Y., 14

Day 0 (Sat, 28.04)

18:00 – 19:00

Excursion in Tartu

(Central square / Raekoja plats)

19:00 – 21:00

Welcome reception, early registration

(University Café, Ülikooli 20)

Day 1 (Sun, 29.04, Dorpat Conference Centre, Turu 2)

08:30 – 09:20

Registration/Opening

09:20 – 10:50

Presentations [Sievers, Tsukerblat, Bussmann-Holder]

10:50 – 11:10

Coffee

11:10 – 12:50

Presentations [Kugel, Seibold, Dzebisashvili, Röhler]

12:50 – 14:00

Lunch

14:00 – 15:40

Presentations [Rosanov, Shepelev, Noatschk, Möller]

15:40 – 16:00

Coffee

16:00 – 17:40

Presentations [Mikheyenkov, Karatsuba, Zolotaryuk, Tsirlin]

17:40 – 19:00

Poster Session

Day 2 (Mon, 30.04, Institute of Physics, W. Ostwaldi 1)

08:30 – 09:00

Bus from hotels to the Institute

09:00 – 10:40

Presentations [Oleś, Lemmens, Stern, Kovaleva]

10:40 – 11:00

Coffee

11:00 – 11:30

Tour in the Institute of Physics

11:30 – 12:45

Presentations [Piazza, Korznikova, Dmitriev]

12:45 – 14:00

Lunch

14:00 – 14:50

Presentations [Silaev, Gabovich]

14:50 – 15:10

Bus (Institute → Museum)

15:10 – 17:00

Excursion: Estonian National Museum

17:00 – 17:20

Bus (Museum → Dorpat hotel)

19:00 – 22:00

Dinner

Day 3 (Tue, 01.05, Dorpat Conference Centre , Turu 2)

09:00 – 10:40

Presentations [Chechin, Archilla, Kosevich, Dubinko]

10:40 – 11:00

Coffee

11:00 – 12:15

Presentations [Janowitz, Sherman, Kuz'min]

12:15 – 14:00

Lunch

14:00 – 15:40

Presentations [Chtchelkatchev, Korovushkin,
Strugovshchikov, Krasnenko]

15:40 – 16:00

Coffee

16:00 – 17:15

Presentations [Chetverikov, Vargunin, Usoltsev]

17:15 – 17:25

Closing