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1 Algorithm Development

Symmetry Enforced Self-Learning Monte Carlo Method Applied to the Holstein Model

Chuang Chen[1,2], Xiao Yan Xu[3], Junwei Liu[3], George Batrouni[4,5,6,7], Richard Scalettar[8], Zi Yang Meng[1,9]
[1]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing, China. [2]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing, China. [3]Department of Physics, Hong Kong University of Science and Technology, Hong Kong, China. [4]Université Côte d'Azur, INPHYNI, CNRS, Nice, France. [5]Beijing Computational Science Research Center, Beijing, China. [6]MajuLab, CNRS-UNS-NUS-NTU International Joint Research Unit, Singapore, Singapore. [7]Centre for Quantum Technologies, National University of Singapore, Singapore, Singapore. [8]Physics Department, University of California, Davis, USA. [9]CAS Center of Excellence in Topological Quantum Computation and School of Physical Sciences, University of Chinese Academy of Sciences, Beijing, China

Self-learning Monte Carlo method (SLMC), using a trained effective model to guide Monte Carlo sampling processes, is a powerful general-purpose numerical method recently introduced to speed up simulations in (quantum) many-body systems. In this work, we further improve the efficiency of SLMC by enforcing the symmetry of the original problem on the effective model. We demonstrate its effectiveness in the Holstein Hamiltonian, one of the most fundamental many-body descriptions of electron-phonon coupling. Simulations of the Holstein model are notoriously difficult due to the combination of the cubic scaling typical of fermionic Monte Carlo and the presence of much longer autocorrelation times than those occurring in the Hubbard model. Our method addresses both these bottlenecks. This enables simulations on large lattices in the most difficult parameter regions, and the evaluation of the critical point for the charge density wave transition at half-filling with high precision.

Boosting convergence of numerical linked-cluster expansions with the Lanczos algorithm

Krishnakumar Bhattaram, Ehsan Khatami
San Jose State University, San Jose, USA

Numerical linked-cluster expansions* have had widespread applications in the exact study of finite-temperature properties of quantum lattice models in the thermodynamic limit. A limiting factor has been the lack of ability to treat increasingly large clusters at high orders in the series exactly using full diagonalization techniques. Here, we show that supplementing the full diagonalization of small clusters in low orders with the partial knowledge of excited states for larger clusters at high orders from the Lanczos algorithm can extend the convergence of the series to lower temperatures than previously possible. We test this approach on the quantum Heisenberg model on a square lattice.

*M. Rigol, T. Bryant, and R. R. P. Singh, Phys. Rev. Lett. 97, 187202 (2006)

DAMAGE ANALYSIS AND DETECTION UNDER VARYING ENVIRONMENTAL AND OPERATIONAL CONDITIONS USING A CHAOS THEORY METHODS: ADVANCED COMPUTATIONAL CODE

Vasily Buyadzhi, Alexander Mashkantsev, Sergey Kirianov, Valentin Ternovsky, Iryna Cherkasova
Odessa State Environmental University, Odessa, Ukraine

One of the important problems in monitoring the engineering (vibrating) structures is problem of analysis, identification and prediction the presence of damages (cracks), which above a certain level may present a serious threat to their performance [1]. The work is devoted to carrying out and advancing effective computational approaches to modelling, analysis and prediction of a chaotic behaviour of structural dynamic properties of the vibrating structures. The computing code developed includes a set of such non-linear analysis and a chaos theory methods as the correlation integral approach, multi-fractal and wavelet analysis, average mutual information, surrogate data, false nearest neighbours algorithms, the Lyapunov's exponents approach, spectral methods and nonlinear prediction (predicted trajectories, neural network etc) algorithms (in versions [2]). As illustration we present the results of the complete numerical investigation of a chaotic elements in time series for the simulated 3DOF system and an experimental cantilever beam, excited by white and pink noise forces [1]. We present firstly computed original data on the Lyapunov's exponents, correlation, embedding, Kaplan-York dimensions, the Kolmogorov entropy. In conclusion, a non-linear prediction method is used for the time series It is shown that even though the simple procedure is used to construct the non-linear model, the results are quite satisfactory.

References: [1]. A. Tjirkallis, A. Kyprianou, Mech.l Syst. Signal Process. 66-67, 282–297 (2016); [2] A. Glushkov et al, Recent Adv. in Computer Engineering, Ed. J.Balicki.(Gdansk, WSEAS Pub.). 21, 143 (2014).

ADVANCED COMPUTATIONAL APPROACH TO STUDYING RYDBERG AND AUTOIONIZATION SPECTRA OF HEAVY ATOMS

Valentin Ternovsky
Odessa State Environmental University, Odessa, Ukraine

The paper is devoted to further development and application of the a relativistic many-body perturbation theory [1] with Dirac-Kohn-Sham (DKS) zeroth approximation combined with the generalized energy approach to studying the spectra and Rydberg and autoionization resonances for heavy atoms, in particular, atoms of lanthanides and actinides (Eu, Tm, Yb, U). The wave function zeroth basis is found from the Dirac equation with a potential, which includes ab initio (the optimized DKS potential, the electric potential of a nucleus). The correlation corrections of the PT high orders are taken into account within the Green functions method (with using the Feynman diagram's technique). All correlation corrections of the second order and dominated classes of the higher orders diagrams (electrons screening, particle-hole interaction, mass operator iterations) are taken into account. To test a new approach we list the experimental (compilation) and theoretical data for energies of YbI singly excited states, namely, data, obtained on the basis of multiconfiguration Hartree-Fock method within the framework of Breit-Pauli relativistic corrections developed by Fischer; data, obtained on the basis of Cowan's relativistic Hartree-Fock method; data of analysis by Wyart-Camus; data by Ivanov et al obtained on the basis of the model many-body perturbation theory and energy approach. A significant part of data for studied elements is received for the first time.

References: [1] A. Glushkov et al, Frontiers in Quantum Systems in Chem. And Physics (Berlin, Springer) 18, 505 (2008); V. Buyadzhi et al, J. Phys.: Conf. Ser. 810, 012047 (2017).

A Comparison of Medium-Sized Basis Sets for the Prediction of Geometries, Vibrational Frequencies, Infrared Intensities and Raman Activities

Brian Ferrari[1], Chris Bennett[1,2,3,4]
[1]University of Central Florida, Department of Physics, Orlando, USA. [2]University of Central Florida, Department of Chemistry, Orlando, USA. [3]Georgia Institute of Technology, Department of Chemistry & Biochemistry, Atlanta, USA. [4]Florida Space Institute, Orlando, USA

Optimized geometries, vibrational frequencies, as well as infrared intensities and Raman activities were calculated for H_2O, NH_3, CH_4, CO, CO_2, HCN, H_2CO, C_2H_2, C_2H_4, and C_2H_6 utilizing popular quantum mechanical levels of theory. Here, density functional theory (DFT) calculations were performed using the B3LYP (Becke, three-parameter, Lee-Yang-Parr) functional, as well as *ab initio* calculations using second-order Møller-Plesset (MP2) perturbation theory and coupled-cluster with single, double and perturbative triple excitations [CCSD(T)] levels of theory were used. We assess and benchmark the performance of 57 different atomic orbital basis sets including various popular families of medium-sized basis sets typically of two to four zeta quality and differing levels of augmentation by polar and diffuse functions. The basis sets range from the commonly adopted Poplestyle (6-31G & 6-311G), Dunning's correlation consistent (cc-pV(n+d)Z & aug-cc-pV(n+d)Z, as well as Truhlar's calendar variations), Jensen's polarization consistent (pc-n & aug-pc-n), Alrich's (def2-...), Sapporo's and Karlsruhe'as well as atomic natural orbitals (ANOs) such as NASA Ames (ANOn), Neese-style, and Roos-style. We also compare several basis sets specifically designed for calculating vibrational and electronic properties, including the Sadlej-pVTZ (and LPol-X families), as well as SNS families of Barone. The results are compared to experimental values where available, or calculationsperformed with 5 or 6 zeta-level (e.g.,

cc-pV6Z). The performance of each family of basis sets are discussed in terms of their accuracy (and pitfalls), as well as computational resource scaling and efficiency.

2 Astrophysics

Effects of Pressure Anisotropy on Solitary Waves in Multi-ion Plasmas

Sijo Sebastian[1], Manesh Michael[2], Chandu Venugopal[2]
[1]Department of Physics, St. Berchman's College, Changanassery 686101, KOTTAYAM, India. [2]School of Pure and Applied Physics, Mahatma Gandhi University, PD Hills 686560, KOTTAYAM, India

Using Reductive Perturbation Technique (RPT), Zakharov-Kuznetzov (ZK) equation is derived for ion acoustic solitary waves in a five component magnetized plasma consisting of hydrogen ions, both solar and cometary origin of electrons and positively and negatively charged heavier pair ions. Both electron components are modeled by Kappa distribution function. The Chew, Golberger-Low (CGL) theory [1] has been included in the derivation to study the combined effect of anisotropic pressure of lighter hydrogen and heavier pair-ions. Various combinations of the anisotropy of the three types of ions have been considered in the numerical study. For parameters relevant to comet Halley [2, 3], it is seen that at lower values of the phase velocity, the width and amplitude of the solitary waves depend strongly on the anisotropy parameters. On the other hand, the width and amplitude of the solitary waves are independent of the anisotropy of the ions.

References

[1] Bashir MF, Behery EE and El-Taibany WF (2015) Effect of anisotropic dust pressure and superthermal electrons on propagation and stability of dust acoustic solitary waves. Phys Plasmas 22: 062112.

[2]Brinca AL and Tsurutani BT (1987) Unusual characteristics of the electromagnetic waves excited by cometary newborn ions with large perpendicular energies. Astron Astrophys 187: 311.

[3] Chaizy P, Reme H, Sauvaud JA, d'Uston C, Lin RP, Larson DE, et al. (1991) Negative ions in the coma of comet Halley. Nature 349: 393.

Study of Thermodynamic Properties of Hydrogen Thermal Plasma in Local Thermodynamic Equilibrium Including Pressure Derivative of Partition Function

Rohit Sharma[1], Kuldip Singh[2], Gurpreet Singh[3]
[1]Satyam Institute of Engineering & Technology, Amritsar, India. [2]Department of Physics, Guru Nanak Dev University, Amritsar, India. [3]Department of Physics, DAV College, Bathinda, Bathinda, India

In present work, thermodynamic properties such as compressibility coefficient, adiabatic coefficient, specific heat at constant volume, isentropic coefficient and sound speed of hydrogen thermal plasma in local thermodynamic equilibrium (LTE) conditions have been examined in the temperature range from 5000K to 50000K at different pressures 1atm, 100 atm and 1000 atm. Two cases have been considered (i) when the expressions include the pressure derivative of partition function and (ii) when pressure derivative of partition function is excluded from expressions. It has been observed that the temperature from which pressure derivative starts influencing a given the thermodynamic property, increases with increase of pressure. The thermodynamic property for the case (i) is always greater than its value for the case (ii) for compressibility coefficient and specific heat at constant volume while reverse is true for adiabatic coefficient, isentropic coefficient and sound speed. The relationship of compressibility coefficient with degree of ionization does depend upon pressure in case (i) where as it is independent of

pressure in the case (ii). The relative deviation between the two cases increases with augmentation of pressure for compressibility coefficient, specific heat at constant volume and adiabatic coefficient such that their maximum values are large whereas for isentropic coefficient and sound speed, it is marginal even at high values of pressure.

X-Ray Source Distribution and the Discovery of 14 New Black Hole Candidates within the Milky Way

Cameron Woo
Independent, Independent, USA

The purpose of this investigation was to identify new black holes in the Milky Way galaxy. Data was gathered from the Chandra Telescope and was analyzed to discover black hole candidates and other source populations. The catalog of 9017 sources was filtered to 5259 usable sources, which were then divided into “hard” and “soft” sources, using the ratio of their high energy to low energy X-rays (referred to as HR2 cuts). They were further subdivided by net counts, flux, variability, and distance. By organizing the sources into log-log plots for flux and distance, separating them into variable and non-variable sources, and using spectral fitting, different populations were distinguished and identified.

The general distribution of X-ray systems throughout the galaxy was determined and the following findings were made: black holes located within the central parsec, predominantly intermediate polars within the central 1-10, then a mix of intermediate polars and dwarf novae eventually leading to a dominance of dwarf novae ranging out from 100 parsecs. Following this, 14 black hole candidates were discovered. This finding dramatically increases the total known black hole candidates within the galaxy, by nearly 25%, and disturbs the current notions of black hole distribution throughout the Milky Way. Future studies could investigate the hard non-variable sources, which were unexplored in this study. Learning of black holes and their locations can give new insight into the Milky way galaxy by allowing further understanding of the interactions and evolutions of celestial bodies.

NuSTAR Search for Black Holes within the Galactic Center

Dong Hoon Lee[1], Michael Chang[2]
[1]St. Andrew’s School, Middletown, USA. [2]Stanford University, Stanford, USA

This investigation reports on the 2016 Nuclear Spectroscopic Telescope Array (NuSTAR) observation of the Galactic Center (GC). Two new transients were identified within the Galactic Center, Swift J174540.7-290015 (Transient 15) and Swift J174540.2-290037 (Transient 37). Having observed the GC for 10 years and detected no prior outburst, it can be concluded that the time between outburst (recurrence time) is longer than 10 years. The recurrence time of a neutron star is less than 10 years, while a black hole’s is assumed to be approximately 100 years. Therefore, it can be concluded that these transients are very likely black hole binaries. Through both spectral fitting and timing analysis, Transients 15 and 37 were identified as black hole candidates. The observed number of transients were used to estimate the existence of 30 black hole binaries within the Galactic Center, 27 still unobserved, indicating the likelihood of a substantive population of black holes within the Galactic Center.

Space Debris Removal Mechanism Using CubeSat with Gun Shot Facilities

Shankar Bhattarai
Tribhuvan University, Kathmandu, Nepal

Space debris is a very perilous problem that cannot be cracked in it, even in the near future. Awkwardly, most of the proposed methods for space debris removal are not successfully serviceable. Keeping in view the limitation of the existing methods for debris removal an active approach is needed in this regard required to be instigated purposefully. More than 12,000 orbiting items in total are regularly tracked by the US Space Surveillance Network and maintained in their catalogue, which covers objects larger than approximately 5 to 10cm in low Earth orbit (LEO) and 30cm to 1m at geostationary altitudes (GEO). This paper proposing linking mostly available technologies in a new way for sifting the space debris. The basic idea is the CubeSat with Gunshot facilities is categorically working to deorbiting the debris. This is certainly an old fashioned but the concept of the CubeSat with Gunshot amenities will be a new environment. In this paper we are proposing an idea to remove space junks in Low Earth Orbit (LEO) using CubeSat with Gunshot equipment. Our target is to confiscate the small junk, which involves different materials of size between the ranges 0.2 to 1 inches. This research intended to comprehend and assess the range of the space debris removal activity in terms of the simple business model.

Keywords: Space Debris, CubeSat,Low Earth Orbit, Gunshot Mechanism

MULTI-PHOTON SPECTROSCOPY OF THE DEBYE PLASMAS ATOMIC SYSTEMS IN A ONE- AND TWO-COLOR LASER FIELDS: ADVANCED COMPUTATIONAL APPROACH

Vasily Buyadzhi, Anna Kuznetsova, Andrey Svinarenko, Alexander Belodonov
Odessa State Environmental University, Odessa, Ukraine

In this paper one-and two-color multi-photon spectroscopy of a number of transitions in a hydrogen, lithium and caesium atoms and ions (free and immersed in a Debye plasmas) is studied theoretically. The computational approach is based on the relativistic energy approach and relativistic operator perturbation theory [1,2]. The plasmas medium screening effects are taken into account by introducing the Yukawa-type electron-nuclear attraction and electron-electron repulsion potentials into the electronic Hamiltonian for N-electron atom (ion) in plasmas [2]. The calculations have been performed for plasmas with the typical corresponding parameters: the Debye lengths l_D=5a.u. (solar core: temperature T=10^7K; density 10^{32} m^{-3}) and 25 a.u. (inertial confinement: temperature T=10^4K; density 10^{28} m^{-3}) . It is calculated variation of the multi-photon resonance enhancement frequencies in a few atomic systems (hydrogen, lithium) in dependence on plasmas parameters. For example, the corresponding values for the resonance enhancement frequencies ω_{r1}, ω_{r2} and ω_{r3} for the 1s–4f transition in the hydrogen for different Debye lengths (l_D=5-50 a.u.) are between 0.009 and 0.023a.u. The hydrogen plasma results are compared with the similar data, presented in [3].

References: [1] A. Glushkov, L. Ivanov, Phys. Lett. A **170**, 33 (1992); E. Ivanova, L. Ivanov, L. Knight, Phys.Rev.A. **48**, 365 (1993); [2] S Malinovskaya, A. Glushkov, O. Khetselius *et al.*, Int.J.Quant.Chem. **111**, 288 (2011); V Buyadzhi, et al, J.Phys.: Conf. Ser. **905**, 012003 (2017); V Buyadzhi *et al*, J.Phys.: Conf. Ser. **810**, 012047 (2017); [3] K.Wang et al, J. Phys. B: At. Mol. Phys. **18**, 4539 (1985).

3 Computational Physics Education

Modification of Bohr's equation for the energy of hydrogen atom

Raji Heyrovska
Academy of Sciences of the Czech Republic, Emeritus, Prague, Czech Republic

Bohr's equation for the ground state energy of hydrogen is half the Coulombic energy, which is negative. As hydrogen is the most abundant element in the Universe, it implies that the energy of the Universe is predominantly negative, which is strange. Therefore, the author replaced the Coulombic energy by electromagnetic energy, which is of the same magnitude but positive. This modification of Bohr's theory gave rise to many interesting results, showing that atom is aunique construction of Nature and that atomic physics is much simpler.

4 Energy, Environment and Climate Modeling

Modeling the Absorption Spectra of Organic Molecules at the Ice-Air Interface

Fernanda Bononi[1], Davide Donadio[2], Ted Hullar[2], Cort Anastasio[2]
[1]UC Davis, California, USA. [2]UC Davis, Davis, USA

Snow packs and tropospheric clouds are important sites for environmentally significant reactions. Among them, the photolysis of organic molecules is of particular importance, as it converts pollutants into more volatile molecules that are then released into the atmosphere. Organic molecules are solvated in the quasi-liquid layer (QLL) at the air-ice interface or in liquid-like regions (LLR) within the ice matrix. Previous work shows that reaction rates for such reactions could be enhanced in the air-ice interface when compared to solution. The bathochromic shift of the UV-vis absorption spectrum may be responsible for such enhancement.[1] Hence it is essential to characterize the solvation shell of such molecules in water and at the air-ice interface at the molecular scale.

Starting from a previously characterized ice model,[2] we used large-scale classical molecular dynamics (MD) to characterize the solvation of phenol and guaiacol at the air-interface and in supercooled water. Smaller models treated at the level of first-principles MD are then used to calculate the absorption spectra of the aforementioned molecules, accounting for the variations within the solvation shell at the QLL at finite temperatures, using time-dependent density functional theory (TDDFT).

The results obtained through these calculations are compared to measurements obtained experimentally in order to optimize and validate model approaches that will be used to provide further insight into the nature of photochemical reactions rate enhancement in snow and ice when experimental measurements are not attainable.

NEW COMPUTATIONAL APPROACH TO THE EARTH ATMOSPHERE LARGE-SCALE PROCESSES AND ANGLE MOMENTUM BALANCE MODELLING: ATMOSPHERIC CIRCULATION, TELECONNECTION AND RADIO-WAVEGUIDES

Alexander Glushkov, Anna Romanova, Yuliya Bunyakova, Andrey Svinarenko, Iryna Buchko
Odessa State Environmental University, Odessa, Ukraine

We present new methods of monitoring the Earth system low-frequency scale processes on the basis of observing some summated contributions of low frequency oscillations for geophysical factors. They base on the energy and angle moment balance relations and new scheme for calculation of the macro-turbulence regime in typical atmospheric processes, which are known as circulation forms [1,2]. The balance analysis allows to predict the large-scaled atmospheric transformations and teleconnection phenomena and to give their quantitative description. We carried out a series of computer experiments at the Pacific ocean region to study global mechanisms in the atmospheric models and check the seasonal sequences of conservation (or disbalance) of the Earth atmosphere angle momentum and to provide new predictors for the long-termed forecasts of the low frequency atmospheric processes. The current function (complex velocity) fields are calculated for typical atmospheric circulation's forms. The experiments allowed quantitatively defining a direct link between an atmospheric turnover and circulation forms through the front divider position and typical low frequency process of conservation of angle moment balance. We adapted modified theory of the macro-turbulence for possible using the atmosphere radio-waveguides as a special effective predictors in long-termed plan.

References: [1]. Glushkov A.V. etal Water resources in Asia Pasific Region.- Kyoto, Japan .-2003.-P.1355-1358; Nonlinear Proc. in Geophys. 11, 285 (2004); [2]. Glushkov A.V., Methods of a Chaos Theory to Complex Geo-Systems, 2012, Odessa, Astroprint; Glushkov A., Khetselius O., Buyadzhi V.V., New Methods of Mathematical Modelling in Earth and Environmental Sciences, 2016, Odessa, OSENU

AN ADVANCED CHAOS-GEPMETRIC COMPUTATIONAL APPROACH TO ANALYSIS, PROCESSING, PREDICTION OF ENVIRONMENTAL MEASUREMENTS DATA: AIR POLLUTION

Olga Khetselius, Vasily Buyadzhi, **Alexander Glushkov**, Anna Romanova, Yuliya Bunyakova
Odessa State Environmental University, Odessa, Ukraine

An advanced chaos-dynamical approach to analysis, processing and forecasting measurement data of the atmospheric pollutant concentrations is presented. It includes a combined group of non-linear analysis and chaos theory methods such as the autocorrelation function method, multi-fractal formalism, wavelet analysis, mutual information approach, correlation integral analysis, false nearest neighbour (FNN) algorithm, Lyapunov's exponents and Kolmogorov entropy analysis, surrogate data method, memory functions, neural networks algorithms. As illustration, the results of computational analysis and processing some air pollutants concentration data are listed In our study, we used the multi-year hourly concentrations measurement data for nitrogen dioxide obtained for several sites of the Gdansk (2003-2004; one year total of 20x8760 data points) and the Odessa (2001-2006; 20x6570 data points). We present the data for Gottwald-Melbourne parameter, the correlation and embedding dimensions, Lyapunov's exponents, Kaplan-Yorke dimension, average limit of predictability (Pr_{max}) for studied time series. The correlation D (attractor dimensions) values are smaller than the dimensions obtained by the FNN algorithm. Some studied time series have the highest Pr_{max} (> 2 days), and other time series have the predictabilities slightly less than 2 days.

References: [1]. Glushkov A V 2012 *Methods of a chaos theory* (Odessa: OSENU); Glushkov A, Khetselius O, Brusentseva S, Zaichko P, Ternovsky V 2014 *Recent Adv in Computer Engineering* (Gdansk: WSEAS) **21** 69; [2] Bunyakova Yu, Khetselius O 2009 *Proc 8th Int Carbon Dioxide Conf* (Jena, Germany) T2-098; Bunyakova Yu, Glushkov A, Khetselius O,et al, 2017 *Sens Electr and Microsyst Techn***14**(3) 65.

5 Fluid Dynamics

NEW COMPUTATIONAL APPROACH TO MODELLING DYNAMICS OF ATMOSPHERE VENTILATION AND INDUSTRIAL CITY'S AIR POLLUTION ANALYSIS

Olga Khetselius, Anna Ignatenko, Anna Romanova, Iryna Buchko, Alexander Glushkov, Andrey Svinarenko
Odessa State Environmental University, Odessa, Ukraine

We present a new effective approach to analysis and modelling the natural air ventilation in an atmosphere of the industrial city, which is based on the Arakawa-Schubert and Glushkov models, modified to calculate the current involvement of the ensemble of clouds, and advanced mathematical methods of modelling an unsteady turbulence in the urban area. The combined the Arakawa-Schubert and Glushkov model includes the budget equations for mass, moist static energy, total water content plus the equations of motion. For the first time the methods of a plane complex field and spectral expansion algorithms are applied to calculate the air circulation for the cloud layer arrays, penetrating into the territory of the industrial city. We have also taken into account for the mechanisms of transformation of the cloud system advection over the territory of the urban area. The results of test computing the air ventilation characteristics are presented for the Odessa, Trieste, Gdansk and New- York cities. All above cited methods and models together with the standard monitoring and management systems can be considered as a basis for comprehensive computational "Green City" technology.

References: 1. Arakava A, Shubert W H 1974 *Journ. of Atm. Sci.***31** 674; 2. Glushkov A V 1999 *Meteorology, Climatology and Hydrology***38** 77; 3. Glushkov A V 2012 *Methods of a chaos theory* (Odessa: Astroprint); 4. Glushkov A V, Khetselius O Yu, Agayar E V, et al 2017 *IOP Conf. Ser.: Earth Environ. Sci.***92** 012014.

6 Lattice Field Theory in Particle and Nuclear Physics

NEW COMPUTATIONAL APPROACH TO HADRONIC ATOMIC SYSTEMS: RADIATIVE AND STRONG INTERACTION CORRECTIONS

Yuliya Dubrovskaya, Larisa Vitavetskaya, Olga Khetselius, Inga Serga, **Valentin Ternovsky**
Odessa State Environmental University, Odessa, Ukraine

We present the relativistic approach to hadronic (pionic) atoms based on the Klein-Gordon-Fock equation with optimized p^--N interaction optical potential and relativistic many-body perturbation theory with Dirac-Breit-Kohn-Sham zeroth approximation Hamiltonian and correct treating radiation, electron-screening, nuclear effects (finite size, quadrupole deformation) effects [1]. It is developed a precise theory for calculating energy levels shifts and widths, provided by a strong p^--N interaction ("strong" width) and the interaction of the pion with QED vacuum (radiation width) within the model optimized optical complex p^--N interaction potential and relativistic energy approach based on the Gell-Mann and Low formalism with complex relativistic e-e interaction potential. For a number of heavy atoms, including, p^-- ^{165}Ho,^{169}Tm, ^{173}Yb, ^{175}Lu, ^{181}Ta, ^{197}Au, ^{203}Tl, ^{208}Pb, ^{209}Bi, there are obtained the values 4f and 3d levels shifts and widths, caused by a strong p^--N interaction, including correction directly related to the effect of nuclear quadrupole deformation. It has been carried out computing energy (electromagnetic) contributions (Coulomb, radiation corrections, incl. polarization of vacuum, such as Uehling-Serber, Wichman-Kroll and Kallen-Sabry ones, Breit-Rosenthal-Crawford-Schawlow effect etc.).

References:

[1] Serga I N, Dubrovskaya Yu V, Kvasikova A S, Shakhman A N, Sukharev D E 2012 *J. Phys.: Conf. Ser.***397** 012013; Glushkov A V 2012 *Progress inTheoretical Chemistry and Physics* (Springer) **26** 231-252; Khetselius O Yu 2009 *Int. J. Quant.Chem*. **109** 3330.

7 Materials Physics

Molecular dynamic study of solid-state transitions of ammonium nitrate

Hongyu Yu, Defang Duan, Kuo Bao, Da Li, Bingbing Liu, Tian Cui
Jilin University, Changchun, China

High-pressure polymorphism and phase transitions have wide ranging consequences on the basic properties of ammonium nitrate. However, the phase diagram of ammonium nitrate at high pressure and high temperature is still under debate. This study systematically investigates the phase transitions and structural properties of ammonium nitrate at a pressure range of 5–60 GPa and temperature range of 250–400 K using ab initio molecular dynamics simulations. Two new phases are identified: one corresponds to the experimentally observed phase IV' and the other is named X. We find that the lattice strains play a significant role in the formation and stabilization of phase IV', which provide a reasonable explanation for recent experiments in which phase IV-IV' transition only appears under nonhydrostatic pressure. In addition, 12 O atoms neighboring the N_H (N atom in ammonium cation) atom are selected as reference system to clearly display the tanglesome rotation of ammonium cation.

Application of Van Der Waals Density Functionals to Two Dimensional Systems Based on a Mixed Basis Approach

Chung-Yuan Ren[1], Yia-Chung Chang[2], Chen-Shiung Hsue[3]
[1]Depart of physics, National Koahsiung Normal University, Koahsiung, Taiwan. [2]Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan. [3]Department of Physics, National Tsing Hua University, Hsinchu, Taiwan

A van der Waals (vdW) density functional was implemented with the charge density obtained by the mixed basis approach previously developed for studying two dimensional systems, in which the vdW interaction plays an important role. The basis functions here are taken to be the localized B-splines for the finite non-periodic dimension and plane waves for the two periodic directions. This approach will reduce the size of the basis set, especially for large systems, and therefore is computationally efficient for the diagonalization of the Kohn-Sham Hamiltonian.

The nonlocal vdW correlation was treated appropriately according to the layered geometry structure.

We applied the present algorithm to calculate the binding energy for graphene and hexagonal boron nitride and the results are consistent with data reported earlier. We also found that, due to the relatively weak vdW interaction, the charge density obtained self-consistently for the whole bilayer system is not significantly different from the simple addition of those for the two individual monolayer systems, except when the interlayer separation is close enough that the strong electron-repulsion dominates. This finding suggests an efficient way to calculate the vdW interaction for large complex systems involving Moire pattern configurations.

Novel superconductivity in ternary hydrides $MAlH_6$ (M= Li, Mg) under high pressure

Yanbin Ma[1], **Defang Duan**[1,2], Ziji Shao[1], Hongyu Yu[1], Da Li[1], Fubo Tian[1], Bingbing Liu[1], Tian Cui[1]
[1]State Key Laboratory of Superhard Materials, College of Physics, Jilin University, Changchun, China.
[2]Department of Materials Science and Metallurgy, University of Cambridge, Cambridge, United Kingdom

Hydrogen-rich materials can be metallized at much lower pressures due to ”chemical pre-compression” and considered as good candidates for high *T*c superconductors. Recently, both of theoretical and experimental reports on sulfur hydrides under pressure exhibiting high T_c with 200 K has inspired further efforts to research the superconductivity in hydrogen-rich materials.

Here, we found two ternary hydrides $LiAlH_6$ and $MgAlH_6$ stabilize above 200 GPa and share a similar tetragonal structure. our investigations suggest that it is H-dominated electrons that couple strongly all phonon modes, which results in large electron-phonon coupling parameters λ = 1.87 and 0.85, and high superconducting transition temperatures T_c of $\tilde{1}$60 and 77 K for $LiAlH_6$ and $MgAlH_6$ at 200 GPa, respectively. Importantly, investigations on $MAlH_6$ also indicates that the improvement of H-derived DOS-FL is a very promising strategy to enhance superconductivity of hydrides, which gives a strong motivation to design and explore some novel high temperature superconductors in other ternary hydrides.

UNRAVELING A NEW HEAT TRANSPORT REGIME AT THE NANOSCALE

Giuseppe Barbalinardo, Shunda Chen, Davide Donadio
University of California, Davis, USA

The understanding of how the thermal properties of a semiconductor change when its size is reduced, besides being a fundamental scientific problem, has a huge technological importance in electronics and thermoelectric energy conversion. Some examples include microelectronics, where using XUV lithography it is possible to produce circuits with characteristic lengths of few tens of nanometers, energy harvesting and conversion, where the efficiency is determined by the heat transferred between the device and the outside environment, and materials science, where newly designed system, like two-dimensional van der Waals materials, are presenting intriguing heat transport properties.

In this work we discuss heat transport in semiconductor nanostructures, overcoming fundamental gaps in the current state the art for numerical methods. Specifically, we have developed a novel approach based on Anharmonic Lattice Dynamics (ALD) and the Boltzmann transport equation, which allows us to calculate thermal transport in nanoscale systems, including a satisfactory treatment of finite size in the direction of the thermal flux at quantum mechanical level. In particular, we address size scales in which phonon transport is in between the ballistic and the diffusive regimes. We validated our approach against molecular dynamics simulations of silicon thin films, silicon nanowires and carbon nanostructures.

A Detailed Numerical Analysis for High-T_c Superconductivity Phase Diagram Based on U(1) Slave-Boson Approach to the *t-J* Hamiltonian

Sul-Ah Ahn[1], Hyeyoung Cho[1], Sung-Ho S. Salk[2]
[1]Korea Institute of Science and Technology Information, Daejeon, Korea, Republic of. [2]Pohang University of Science and Technology, Pohang, Korea, Republic of

One of the major theoretical challenges in high-T_c superconductivity is to reproduce the observed phase diagrams which display the monotonously decreasing pseudogap temperature and the dome shaped superconducting transition temperature in the plane of temperature vs. hole concentration. Earlier Lee and Salk [Phys. Rev. B **64,** 052501 (2001); ibid. **71**, 134518 (2005)] reported a successful reproduction of the phase diagram by introducing a realistic slave-boson approach to the Heisenberg term in the *t-J* Hamiltonian. More recently, Shin et.al. [J. Supercond. Nov. Magn. **23**, 637 (2010)] presented both the temperature and the doping dependencies of magnetic susceptibility and spin pairing correlations involved with spin dynamics in high-$T_c$superconductivity in good agreement with measurements. Most recently, Salk [Quantum Studies: Mathematics and Foundations**5**, 149–159 (2018) presented a comprehensive study of high temperature superconductivity based on the well predicted phase diagram mentioned above and a possibility of room temperature superconductivity revealing the higher, the antiferromagnetic coupling constant J, the higher, the superconducting transition temperature Tc. Here we discuss a hither-to-unreported detailed numerical analysis of the phase diagram by varying the values of J, specifically paying attention to our U(1) slave-boson approach [Phys. Rev. B 64, 052501 (2001)] to the *t-J* Hamiltonian. For the sake of convergence test, we vary lattice size from 10x10 to sufficiently larger sizes, we find that the lattice size of 20x20 shows good agreement with any higher lattice sizes we tested, revealing excellent agreement with the observed tendency of phase diagrams of Cu-based high temperature superconductors

Numerical simulation of resonant inelastic x-ray scattering: a Wannier-orbital based method

Chunjing Jia
SLAC, Menlo Park, USA

As a fast developing spectrospic methods, resonant inelastic x-ray scattering (RIXS) have been employed in the study of a broad range of areas including physics, materials science and chemistry etc. The incident and outgoing photon energies, light polarizations and momentum transfers can provide us with rich information such as electronic structure, collective excitation, charge transfer, correlation effect and so on. However, we lack of a general theory to simulate RIXS spectra for both localized (such as cuprates and transition-metal complexes) and itinerant systems (weakly correlated systems where the electronic hybridization between neighboring or short-range atoms are important, so that the band dispersion contributes a lot to the RIXS spectra). Here we present a newly developed Wannier-orbital based method for RIXS simulation. This method works well in terms of both calculational efficiency and precision in predicting RIXS spectra for weakly correlated systems where the band physics dominates. Since this method is based on Wannier-orbital, it has a natural connection to the cluster multiplet method to treat the strongly correlated systems. In this presentation, we will discuss the numerical method, as well as compare the simulation results with RIXS experiments for selected materials.

Quantum transport in driven networks of harmonic oscillators

Doniyor Babajanov[1], Hikmat Matyoqubov[2], Davron Matrasulov[1], Jambul Yusupov[1]
[1]Turin Polytechnic University in Tashkent, Tashkent, Uzbekistan. [2]Urgench State University, Urgench, Uzbekistan

Particle and wave transport in networks is of importance for broad variety of problems in condensed matter physics, polymers, optics and biophysics. In case of submicron scales wave dynamics in networks can be described in terms of so-called quantum graphs. In this work we address the problem of a driven quantum graphs by considering, as the driving force, parabolic wells. In other words, we study network of quantum harmonic oscillators by solving the stationary Schrodinger equation on metric graphs in the presence of harmonic oscillator potential with bond-dependent frequency. Such network of quantum harmonic oscillators can be used for modeling of vibrations in discrete or branched systems, such as crystal lattices, molecular chains, polymers, etc. Our approach for the study of quantum harmonic oscillator network is based on considering it as a set of confined harmonic oscillators connected at vertices. Confined, or bounded harmonic oscillator presents parabolic potential given at finite interval. To solve Schrodinger equation on harmonic oscillator network we impose for confined harmonic oscillator wave functions the vertex boundary conditions providing continuity of wave function and Kirchhoff rule at the vertex.

For such boundary conditions we explore wave packet dynamics and optical conductivity of system and reveal the conditions for transparent (reflectionless) wave transmission through the network branching points.

Pressure-Induced Superconducting Ternary Hydride H_3SXe: A Theoretical Investigation

Da Li, Tian Cui, Fubo Tian
JiLin University, ChangChun, China

Generally, heavy elements only contribute the acoustic phonon modes, which are less important for the superconductivity of hydrides. However, we found that the heavier elements have the ability to enhance the phonon-mediated superconductivity in ternary hydrides. In the H_3S–Xe system, a novel H_3SXe compound has been found by first principle calculations. The structural phase transitions of H_3SXe under high pressures have been studied. The *R*-3*m* phase of H_3SXe has been predicted to appear at pressures above 80 GPa, then further transitions to *C*2/*m*, *P*-3*m*1 and *Pm*-3*m* phases at pressures of 90, 160 and 220 GPa, respectively. The *Pm*-3*m*-H_3SXe with the similar structural feature of *Im*-3*m*-H_3S is predicted to be a potential high-temperature superconductor with the T_c of 89 K at 240 GPa. The 'H_3S' host lattice of *Pm*-3*m*-H_3SXe plays a crucial role in influencing the T_c value. Although the T_c value of H_3SXe is lower than that of H_3S at high pressure, the Xe atoms have the capability to accelerate the hydrogen-bond symmetrization. In the H_3S–noble gas elements system, the linear increase of T_c values with the increasing of atomic number, indicating the superconductivity can be modulated by changing the relative atomic mass of noble gas elements.

Enhancement of Quantum Capacitance by Chemical Modification of Graphene and ZigzagGraphene Nano-ribbon Supercapacitor Electrodes: A First PrincipleCalculation.

SRUTHI T, DR KARTICK TARAFDER
NATIONAL INSTITUTE OF TECHNOLOGY, MANGALORE, India

Graphene-based materials have been proposed as promising electrodes for super capacitors. Recently, it has been found that the main limitation of these electrodes is their low quantum capacitance, which is a direct result of the shortage states near the Fermi level. Using first principle density functional theory calculations, this work explored the variation in electronic structure and the quantum capacitance of chemically modified graphene and zigzag graphene nanoribbon(ZGNR). Chemical modifications of zigzag graphene nanoribbons with different adatom concentration and width terminations were tried to enhance the quantum capacitance. We compared the quantum capacitance of pristene graphene and ZGNR with different adatoms on all possible positions. Our results clearly shows that the number of adatom containing groups and thelocation of adatom region largely influence the electronic properties of graphene nanoribbon and thus the quantum capacitance, when compared to pristine graphene. Our work highlights the importance of the quantum capcitance in the overall performance of graphene - based super capacitors. Quantum capacitance calculations confirmed the greater advantage of some chemically modified graphene compared with those pristine graphene. This work suggests the possibility to enhance quantum capacitance of the graphene - based electrodes using the effect of chemical modification and suggests that 2D graphene and ZGNR are promising electrodes for supercapacitor applications.

Defect levels induced by double substitution of B and N in 4H-SiC: a hybrid density functional study

Emmanuel Igumbor, Walter Meyer
University of Pretoria, Pretoria, South Africa

Electrically active induced energy levels in semiconductor devices could be beneficial to the discovery of an enhanced p or n-type semiconductor. Nitrogen (N) implanted into 4H-SiC is a high energy process that produced high defect concentrations which could be removed during dopant activation annealing. On the other hand, boron (B) substituted for silicon in SiC causes a reduction in the number of defects. This scenario leads to a decrease in the dielectric properties and induced deep donor and shallow acceptor levels. Complexes formed by the N, such as the nitrogen-vacancy centre, have been reported to play a significant role in the application of quantum bits. In this report, results of charge states thermodynamic transition level of the N and B double substitutions in 4H-SiC are presented. The energy of formation and thermodynamic charge state transition levels were predicted. The substitutional complexes are stable with respect to their binding energies. Whereas the impurities located at the C sites induced shallow defect levels, B and N located at Si sites induced only deep defect levels. Under equilibrium conditions, defects are more energetically favourable when the B and N are located at the C sites compare to when located at the Si atomic sites.

Computational Analysis of Au_nV(n=1-8) Nanoalloy Clusters Invoking Density Functional Theory Based Descriptors

Prabhat Ranjan, Tanmoy Chakraborty
Manipal University Jaipur, Jaipur, India

The geometrical, electronic and optical properties of Au_nV (n=1-8) nanoalloy clusters have been investigated invoking Density Functional Theory (DFT) based descriptors. Conceptual DFT based global descriptors have been used to exhibit experimental properties qualitatively. In this report, the experimental properties of Au_nV (n=1-8) nanoalloy clusters are correlated in terms of DFT based descriptors viz., HOMO-LUMO energy gap, Hardness, Softness, Electronegativity, Electrophilicity Index and Dipole Moment. The doping of single vanadium atom in gold clusters enhances the stability of gold clusters and also display pronounced odd-even oscillation behaviours. The computed bond length of instant clusters is numerically close to experimental data. The linear regression analysis has been done in terms of the correlation between our computed descriptors and their experimental counterparts. The high value of linear regression supports our analysis.

Computer simulation of the interaction of fullerene with carbon clusters C_n (n=3-6)

Abdiravuf Dzhurakhalov[1], Ishmumin Yadgarov[2], Vasiliy Stelmakh[2]
[1]Department of Mathematics and Computer Science, University of Antwerp, Antverpen, Belgium. [2]Institute of Ion-Plasma and Laser Technologies, Tashkent, Uzbekistan

Using energy minimization method the stable structures of both freestanding fullerene (C_{60}) and freestanding carbon clusters C_n (n=3-6) were found. For description of the interatomic potential we used Brenner interatomic potential [1], which is specifically parameterized for the carbon systems. Then by the same energy minimization method and using the same Brenner potential, computer modeling of the interaction of fullerene with carbon clusters was carried out.

The results of computer simulations, the various structural changes of both fullerene and of carbon clusters caused by their interaction and binding energies of these formed structures are presented and discussed.

1. D.W. Brenner, O.A. Shenderova, J.A. Harrison, S.J. Stuart, B. Ni, S.B. Sinnot, J. Phys: Condens. Matter 14, 783 (2002).

Ab Initio Investigation of Electronic Properties and Lattice Thermal Conductivity of Zincblende Indium Nitride (InN)

Ibarhim Buba Garba[1], Lawan Sani Taura[2]
[1]Department of Physics, Federal University Gashua, Gashua, Nigeria. [2]Department of Physics, Jigawa State University, Kafin Hausa, Nigeria

The group III nitrides semiconductors (AlN, GaN and InN) are currently investigated due to their promising application in short-wavelength electroluminescence and high-power electronic devices. A very important aspect in the development of these devices is their electronic structure and transport proper-

ties. Amongst the group-III nitrides, InN and its ternary alloys are the least explored. Electronic structure calculations based on Density Functional Theory (DFT) have been extensively used to study and to describe properties of many condensed matter systems. In this work, we have utilized DFT and Boltzmann Transport Equation (BTE) within the Single time Mode Approximation (SMA) to study the electronic and thermal transport properties of InN in zincblende phase. We also determined the temperature dependence of its lattice thermal conductivity and the results were compared with both previous theoretical calculations and experimental measurements.

Chemical and Mechanical pressure dependence of structural, magnetic and electronic properties of $BaFe_2As_2$: Density functional study

Mahdieh Aghajani[1], Hanif Hadipour[2], Mohammad Akhavan[1,3]
[1]Magnet Research Laboratory (MRL), Department of Physics,Sharif University of Technology, Tehran, Iran, Islamic Republic of. [2]Department of Physics, University of Guilan, Rasht, Iran, Islamic Republic of. [3]Center of Excellence in Complex Systems and Condensed Matter, Sharif University of Technology, Tehran, Iran, Islamic Republic of

In the experimental studies of mechanical and chemical pressure effects of $BaFe_2As_2$ there are some discrepancies in the reported pressure range for structural, magnetic and superconducting transitions. Many theoretical works have been done to investigate the electronic structure of these systems, especially in the low pressure range. Nevertheless, more detailed studies at high pressures are needed. We have studied the pressure-induced structural, magnetic and electronic properties of $BaFe_2As_2$ compound in the frame work of density functional theory using pseudopotential Quantum Espresso code within the PBE-GGA parameterization. The chemical pressure effects have been investigated and corresponding results have been compared with the mechanical pressure. The calculated total energy as a function of the unit cell volumes related to compressive pressures have been fitted to get the equilibrium properties. Also, we have found a magnetic transition at the same unit cell volume, around 81 $Å^3$ for the Ba and Ca compounds. Hence, it predicts a magnetic transition pressure of 12 GPa for $SrFe_2As_2$. The structural parameters of $FeAs_4$ tetrahedra are obtained after ionic relaxation and compared with the existing experimental results. The change of these internal parameters is resulted to pressure induced charge transfer; i.e. as the As-*Ae* (*Ae*=Ba, Sr, Ca) bonds absorb electrons, the Fe-As bonds are depleted, and thus the number of holes in Fa-As layers increases. The changes of density of states, band structure and the hole- and electron- pockets of Fermi surface by pressure are discussed.

First principles investigation of transition-metal complexes for battery application

Asif Iqbal Bhatti[1], Olivier Le Bacq[2]
[1]SIMAP, Grenoble INP, Univ. Grenoble Alpes, BP 75, 38402 Saint Martin d'He'res, Grenoble, France. [2]SIMAP, UMR 5266 CNRS-Grenoble INP-UJF, Univ. Grenoble Alpes, BP 75, 38402 Saint Martin d'He'res, Grenoble, France

Standard redox potentials for cathode materials have been investigated using First Principles calculations. We study mono and binuclear transition-metal (TM) complexes $[M(dmbpy)_i]^{n+}$ nX, with three metal centers: Fe, Ru, and Cu. Our modeling at present is validated on mononuclear compounds. This

approach consists in determining the best small polymer (binuclear) made out of these monomers for a battery application. For that, we varied the three available degrees of freedom i.e., the nature of the central TM atom (Fe, Ru, and Cu), counter-ions ($TFSI^-$, PF_6^-, ClO_4^-) in interaction with the polymer and the length of the alkyl chain that connects both mononuclear in the binuclear compound. The Iron compound with alkyl chain length, $-(CH_2)_6-$, is found to be the best candidate with PF_6^-/ ClO_4^- counter-ions. The $[Cu(dmbpy)_2]^{n+}$ nX complex shows too much structure deformation upon loading, making it less reliable for the cathode material.

External field dependences of local magnetic fields in single crystals of Fe_3O_4: a Maximum-Entropy μSR study.

C Morante, E Ghorbani, C Boekema
San Jose State University, San Jose CA, USA

The internal fields in single crystals of magnetite (Fe_3O_4) have been previously studied through muon-spin rotation (μSR). [1] By Maximum-Entropy (ME) μSR, [2] we have analyzed μSR data of single crystal Fe_3O_4 data with external field B parallel to the <111>, <110> or <100> axis. We optimize the ME signal-to-noise ratio by varying the filter time. [2] Several μSR time series indicate a beat pattern. By curve fitting [1] and confirmed *with improved precision* by MEμSR second frequency signals are observed in the temperature range above the Verwey transition (T_V). Assuming one demagnization field and one muon-probe-site set, we find for room temperature (RT) <111> Fe_3O_4 fields larger than the maximum allowable. [1] For <110> at RT Fe_3O_4, hints of secondary fields are seen. We compare our RT B-dependent results with those observed for 205K <110> Fe_3O_4[3] to better understand a transition observed at twice T_V. The existence of these secondary signals may be related to phonon-assisted 3d-electron hopping. [3, 4] Another possibility could be the existence of (magnetically) different muon-probe sites. Our MEμSR B-dependent studies lead to a better understanding of the local magnetism and conduction mechanism in this Mott-Wigner glass. [1, 4]

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[1] C Boekema *et al*, Hpf Interactions 31 (1986) 487; Phys Rev B31 (1985) 1233.

[2] C Boekema and MC Browne, MaxEnt 2008, AIP Conf Proc #1073 p260.

[3] C Morante *et a*l, APS Bulletin, March 2018. [4] C Boekema *et al*, Proc 11th Int M2S Conf (2015).

Thermodynamic model of the laser beam distribution analysis system based on matrix of piezoelectric crystals

Aleksey Pigarev[1], **Vladimir Fedorov**[1], Timur Bazarov[1], Kirill Zotov[1], Oleg Ryabushkin[1,2]
[1]Moscow Institution of Physics and Technology, Dolgoprudnyy, Russian Federation. [2]Kotelnikov Institute of Radioengineering and Electronics, Fryazino Branch, Russian Academy of Sciences, Fryazino, Russian Federation

High-power lasers are widely used for manufacturing and material processing. In such applications it is crucial to control the laser beam quality and its intensity distribution. Conventional methods based on usage of CCD cameras require strong attenuation due to the low optical damage threshold and a relatively narrow operational wavelength range. We have recently introduced a novel method of optical image registration using matrix of piezoelectric crystals. This technique allows measurement of the beam profile without using the attenuation systems even at high power levels of the incident radiation. Each element of the matrix is a tiny crystal piezoelectric resonator that has its own set of the eigenmodes, which frequencies strongly depend on temperature. Following the inverse piezoelectric effect, the eigenmodes are excited noncontactly via the application of the radiofrequency electric field when its frequency is one of the crystal eigenfrequencies. Due to the residual optical absorption each element is heated in compliance with the incident radiation power. The temperature calibration of the piezoelectric resonance frequencies in the uniform heating conditions allows determination of the temperature of matrix elements during its irradiation.

In the present work we have considered the problem of calculating the intensity distribution of an incident radiation using the experimentally measured heating temperatures of the matrix elements as the previous model of the heat insulated elements did not provide sufficient accuracy. The heat conduction equation was solved assuming the heat exchange between the elements. FEM stationary analysis provides connectivity matrices between temperatures and intensity maps.

Sodium Ion Conduction in Germanium Phosphide and Germanium Arsenide

Miqdad Raza[1], Shunda Chen[1], Kirill Kovnir[2], Sabyasachi Sen[1], Davide Donadio[1]
[1]University of California, Davis, Davis, CA, USA. [2]Iowa State University, Ames, IA, USA

The discovery of graphene has sparked much interest in the study of layered materials. Herein, we study the intercalation of sodium in two germanium based layered materials: germanium phosphide (GeP) and germanium arsenide (GeAs) for ion conduction. This material would be viable as a solid-state electrolyte for sodium-ion batteries. For decades, the state-of-the-art has been lithium ion batteries (LIB). But, with a growing need for energy storage and applications, such as electric vehicles (EVs), power tools, and the storage of renewable energy, new battery materials have to be studied, which would allow to replace lithium with more abundant and safer elements, e.g. sodium. Both GeP and GeAs, in their layered forms, have a Gallium Telluride (GaTe)-like monoclinic crystal structure. The layers are bound together by weak van der Waals (vdW) interactions. The interlayer vdW gap provide promising sites for metal intercalation and diffusion. The intercalation of sodium is modeled using first principle calculations. To account for the vdW interactions, a non-local vdW functional is used, which has shown to be more accurate than traditional generalized gradient approximated functionals. All first principle calculations are performed using the Quantum Espresso code. We compute adsorption energies and diffusion barriers at various concentration of Na, and we characterize the structural and electronic properties of the intercalated materials. Preliminary results show a great promise for sodium ion conduction in these materials.

In silico synthesis of monolayer B_3N_3-doped graphene with high thermoelectric power

Thanh Cuong Nguyen, Susumu Okada
University of Tsukuba, Tsukuba, Japan

Based on the density functional theory simulations, we design a novel B_3N_3-doped graphene sheet based on the bottom-up synthesis approach, in which BN-phenanthryne molecules are used as building-blocks. The B_3N_3-doped graphene sheet is a semiconductor with a direct band-gap of 0.64 eV. On the other hand, we also find that the B_3N_3-doped graphene sheet exhibits large thermopower factor of 5.8 (mW/mK^2) at room temperature, comparable to that of commercial Bi_2Te_3 (4 mW/mK^2). This large thermopower could be ascribed to the large density of states near the valence and conduction band edges of B_3N_3-doped graphene. These findings demonstrate that B_3N_3-doped graphene is a promising atomic-layer material for thermoelectric devices.

Thermal Transport Across Graphene Step Junctions

Charles Sievers, Davide Donadio
UC Davis, Davis, USA

Low dimensional materials, such as graphene and carbon nanotubes, have the highest thermal conductivity, which makes them a promising substrate for heat dissipation in nanoscale electronics. Interfaces play a crucial role in determining the thermal dissipation performances in microelectronic systems and thermal resistance. While it is now well established that graphene has an extremely high in-plane thermal conductivity, the thermal energy flow at multi-layer graphene junctions, and at the interfaces between graphene layers and bulk substrates remains mostly unresolved.

Here we consider a two-to-one layer graphene junction, either suspended or supported on silica, for which experimental measurements reported very low thermal conductance. In quantitative agreement with experiments, molecular dynamics and lattice dynamics calculations show that the thermal conductance is one order of magnitude smaller than that of a suspended single graphene sheet, and it stems from the weak interaction between the layers in the bilayer part of the junction.

Thermal conductance is further reduced by 30% upon addition of silica substrate due to interference of graphene flexural modes with the substrate. These modes are the major heat transmitting modes and are unaffected by changes in junction surface area. These results show promising ways in which we can modulate thermal dissipation through layered 2D material junctions.

8 Novel Hardware and Software Paradigms

Self-Consistent Simulation of Dust-Plasma Interactions in a Complex Plasma

Dustin Sanford, Lorin Matthews, Truell Hyde
CASPER, Waco, USA

A complex (dusty) plasma consists of ions, electrons, and micron-sized solid particles, commonly referred to as dust. An interesting aspect of complex plasma is its ability to self-organize into dust liquids, 2D and 3D dust crystal lattices and 1D dust chains. The resulting interaction between the dust and the flowing plasma creates an ion wakefield, downstream from the dust, with the resulting positive space region modifying the interaction between the grains and contributing to the observed dynamics and equilibrium structure of the system. Here we present a molecular dynamics simulation capable of resolving the dynamics of extended dust chains on both ion and dust particle time scales. A two-step leapfrog integration method is used to calculate the trajectories of positive ions and dust particles. Different boundary conditions are employed to model the dust-plasma interactions within the ground-based glass box experiment at CASPER and the PK-4 experiment on-board the ISS. The results are compared with the paired experimental studies.

9 Quantum Many-Body Physics

Tunable refrigeration properties of Rashba coupled nano-junction devices

Priyadarshini Kapri, Saurabh Basu
Indian Institute of Technology Guwahati, Guwahati, India

We propose a tunable nanoscale thermoelectric cooling device based on a metal - insulator - superconductor (MIS) junction in presence of Rashba spin-orbit coupling (RSOC) at ultra-low temperatures and investigate its working principle and performance via a modified version of the Blonder - Tinkham - Klapwijk (BTK) theory. The temperature range for applications of this device is set by the transition temperature (T_c) of the superconducting lead. A challenge in the operational aspects is posed by the fact that the refrigeration properties is restricted to a very narrow range of biasing voltage and lies in the vicinity of the value for the superconducting gap parameter. This means that a control on the operating voltage can be achieved by a careful choice of the superconducting lead. A further tunability of this nano-junction device with regard to its refrigeration properties can be achieved by experimentally achievable manipulative techniques that can tune the value of the Rashba coupling strength as the thermal current that tunnels through the junctions is very sensitive to the RSOC parameter. We have numerically computed the thermal current through this junction and the coefficient of performance and investigated the interplay of the RSOC term and an effective barrier potential, the latter solely being the property of the insulating region. This interplay plays a decisive role in determining the extent of the thermoelectric cooling. These results should have potential importance to the experimental success of refrigeration applications using junction devices and hence veer the applications of nano-structured materials.

Tunneling Dynamics of interacting bosons in a quantum seesaw potential

Sunayana Dutta[1], Pankaj Kumar Mishra[1], Budhaditya Chatterjee[2], Saurabh Basu[1]
[1]Indian Institute of Technology Guwahati, Guwahati, India. [2]Indian Institute of Technology Kanpur, Kanpur, India

We investigate the tunneling dynamics of interacting bosons confined in a driven double well potential. The relative tilt between the wells is varied periodically hence emulating a quantum seesaw. We consider a few boson system which is solved using Multi-configurational time-dependent Hartree method for bosons (MCTDHB) approach via MCTDHX numerical package. Amplitude of driving potential biases the seesaw and provides a handle to investigate the dynamics of bosons in the oscillating environment. For harmonic driving, at small values of the driving amplitude, the dynamics of the particles become very slow rendering a stationary-like state. Hence the trajectory is restricted to a limited region in the dynamical phase space. For intermediate values of driving, the dynamics become periodic in nature, implying that the bosons populating the wells periodically. Dynamics turn completely random accompanied by fast oscillations while driving amplitude increases further. However, when we introduce a chirped modulation to the driving frequency, the temporal evolution of seesaw becomes faster in certain frequency ranges. The tunneling dynamics in such cases, for small amplitudes, show appearance of quasiperiodicity (consist of both slow and fast oscillations). Increasing driving amplitude further, we observe that dynamics, although being periodic, becomes severely damped in amplitude. Our study establishes that by tuning the temporal evolution of quantum seesaw, a precise control on tunneling

dynamics of the correlated bosons can be achieved. Since harmonic driving and chirp frequency modulation of the seesaw are experimentally achievable, such computational exercise can have physical realization in laboratories dealing with cold atomic gases.

Symmetry enhanced first-order phase transition in a two-dimensional quantum magnet

Bowen Zhao[1], Phillip Weinberg[1], Anders Sandvik[1,2]
[1]*Boston University, Boston, USA.* [2]*Institute of Physics, Chinese Academy of Sciences, Beijing, China*

Theoretical descriptions of quantum phase transitions have indicated the existence of critical points with higher symmetry than those of the underlying Hamiltonian. Points of emergent symmetry have not been expected at discontinuous (first-order) transitions, however. Here we present such an example, where phase coexistence at a first-order transition takes the form of an enhanced rotational symmetry in a space of two order parameters. Using quantum Monte Carlo simulations to study a two-dimensional (2D) S=1/2 quantum magnet hosting the antiferromagnetic (AFM) and plaquette-singlet solid (PSS) states recently detected in SrCu2(BO3)2, we observe that the O(3) symmetric AFM order and the Z2 symmetric PSS order form an O(4) vector at the transition. The control parameter (a coupling ratio) rotates the vector from the AFM sector to the PSS sector, with the length of the combined order parameter vector always remaining non-zero. This phenomenon should be observable in neutron scattering experiments on SrCu2(BO3)2.

Translationally transformed coupled-cluster theory in a local basis for periodic systems

Boris Daniel Gutiérrez Cortés, Anthony Dutoi
University of the Pacific, Stockton, USA

There are a lot of interesting problems in surface chemistry where quantum chemistry could give great insight, like reaction mechanisms in heterogeneous catalysis, the effect of surface functionalization on semiconductors, or the influence of defects on the reactivity of crystal surfaces.

Plane wave based methods applied to crystals cannot handle problems that are localized in nature like surface defects and adsorbates. On the other hand, molecular electronic structure techniques, which describe these effects and the locality of the electronic correlation well, are too computationally expensive to use on these systems.

A new approach based on coupled-cluster (CC) theory is proposed. This scheme uses primitive operators that incorporate the periodicity of crystals *and* the locality of electronic interaction. This avoids the calculation of redundant amplitudes. Perfectly periodic surfaces are envisioned as reference wavefunctions for localized defects and chemical reactions.

The working equations are derived starting from the amplitude equations of conventional CC on an infinite system and rearranging them such that the distance to an anonymous cell is an explicit degree of freedom. The formally infinite summations can be truncated by systematically neglecting numerically insignificant amplitudes.

The theory and the details of the computer implementation will be presented, as well as first tests of the

equations on 1-dimensional electronic systems.

Learning Thermodynamics of the Transverse Field Ising Model

Kristopher McBrian, Ehsan Khatami
San Jose State University, San Jose, USA

It has been shown that restricted Boltzmann machines (RBMs) can be trained to learn thermodynamics of classical Ising models or represent the ground state of simple quantum magnetic models such as the transverse field Ising model. Here, we demonstrate that an RBM can also be trained through unsupervised learning to act as a generative model for any excited state of the transverse field Ising model and explore the possibility of training RBMs to produce thermodynamics of the quantum system.

Full counting statistics in the two-dimensional Hubbard model

Stephan Humeniuk
Beijing National Laboratory of Condensed Matter Physics and Insitute of Physics, Chinese Academy of Sciences, Beijing, China

Full counting statistics on a subsystem, i.e. eigenvalue distributions obtainable from repeated projective measurements, are presented for the particle number and (staggered) magnetization in the Hubbard model, which has recently been realized with ultracold atoms under a quantum gas microscope.

While at high temperature the order parameter distribution is Gaussian, for low enough temperature, the distribution of the staggered magnetization at half filling has a shape characteristic of a three-component order parameter, fluctuating mainly in its orientation rather than its length, which is consistent with a description through the non-linear σ-model.

A generalization of the method presented in Ref. [1] allows to compute the full counting statistics also for observables that are quartic in fermionic operators such as the number of doubly occupied sites, holes or magnetic moments on a subsystem. These quantities have become experimentally accessible through a special imaging technique for doubly occupied sites [2], which circumvents the particle loss through light-assisted collisions.

Furthermore, joint probability distributions can be computed by introducing additional counting fields into the generating function. Starting from the single-particle Green's function in momentum space, all details of the method [1] carry over to the computation of the eigenvalue distribution of observables in momentum space, which are accessible in cold atoms experiments in time-of-flight (projective) measurements.

[1] S. Humeniuk and H. P. Büchler, Phys. Rev. Lett. 119, 236401 (2017).

[2] D. Mitra et al., Nature Physics 14, 173-177 (2017).

ADVANCED COMPUTATIONAL APPROACH IN LASER ELECTRON-GAMMA-NUCLEAR SPECTROSCOPY OF ATOMS: “SHAKE-UP” AND NEET EFFECTS

Olga Khetselius
Odessa State Environmental University, Odessa, Ukraine

A new class of problems in computatioonal atomic optics (spectroscopy) is connected with modelling the cooperative laser-electron-nuclear phenomena such as the electron shell shake-up and NEET or NEEC (nuclear excitation by electron transition or capture) effects in heavy atomic systems [1-5]. We present consistent, relativistic computational approach to comupting probabilities of different cooperative laser electron-gamma-nuclear processes in the MCI. The theory is based on the relativistic energy approach (S-matrix formalism of Gell-Mann and Low) and relativistic many-body perturbation theory [2,5,6]. We firstly present new data about intensities of the electron satellites in gamma-spectra of nuclei in neutral (low lying transitions) and O-, F-like MCI for Fe,Cs,Yb atoms, which show an existence of new effect of giant increasing electron satellites intensities at transition from the neutral atoms to the corresponding MCI. We develop an advanced energy approach to the NEET (NEEC) process in heavy MCI and list values of NEET probabilities in nuclei of Os,Ir,U,Mt,Au of O-and F-like MCI. The data listed demonstrate an effect of the significant changing NEET probabilities under transition from the atomic/nuclear systems to MCI.

References:

1. Ivanov L, Letokhov V 1987 *JETP*. **93** 396.
2. Glushkov A, Khetselius O, Malinovskaya S 2008 *Europ.Phys.J.***T160** 195
3. Tkalya E 2007 *Phys.Rev.A.***75** 022509
4. Palffy A, Harman Z and Scheid W 2006 *Phys. Rev.A***73** 012715
5. Khetselius O 2013 *Progress inTheor. Chem. & Phys.* (Springer) **26** 217-230
6. Khetselius O 2009 *Int. J. Quant.Chem*. **109** 3330

COMPUTING HYPERFINE STRUCTURE OF HEAVY ATOMS AND MULTICHARGED IONS WITHIN OPTIMIZED RELATIVISTIC MANY-BODY PERTURBATION THEORY

Olga Khetselius, Olga Antoshkina, Dmitry Mironenko, Tatyana Tkach
Odessa State Environmental University, Odessa, Ukraine

In the paper an effective ab initio relativistic many-body perturbation theory formalism [1-3] with an accounting for the relativistic, correlation, nuclear, radiative effects is applied to computing the hyperfine structure (hfs) parameters for heavy atoms (Cs, Pb, Fr) and multicharged (Li-like) ions. The important point is using a generalized relativistic dynamical effective field nuclear model and the optimized one-quasiparticle representation in the theory of the relativistic atomic systems [4]. There have taken into account all correlation corrections of the second order and dominated classes of the higher orders diagrams. The magnetic inter-electron interaction is accounted in the lowest (on α^2 parameter, α is the fine structure constant), the Lamb shift polarization part - in the Uehling-Serber approximation, self-energy part is accounted effectively within the Ivanov-Ivanova non-perturbative procedure [5]. The hfs energies and constants, derivatives of the one-electron characteristics on nuclear radius, electric, magnetic moments for some Li-like ions are calculated. The detailed analysis of the data and comparison with available theoretical and experimental data (see [5,6] and Refs. therein) is performed.

References [1] A. Glushkov *et al.*, Nucl. Phys. A **737**, 21 (2004). [2] O. Khetselius, Phys. Scr. T **135**, 014023 (2009). [3] O. Khetselius, I. J. Quant. Chem. **135**, 014023 (2009). [4] A. Glushkov *et al.*, Prog.Th.Ch. Phys. **22**, 51 (2011). [5] E. Ivanova *et al.*, Phys. Rep. **164**, 315 (1988). [6] V. Yerokhin *et al.*, Phys. Rev. A **75**, 062501 (2007).

ADVANCED COMPUTATIONAL APPROACH TO HEAVY ATOMS AND NUCLEI IN A STRONG LASER FIELD:DC, AC STARK EFFECT, MULTIPHOTON RESONANCES

Alexander Glushkov, Anna Kuznetsova, Anna Buyadzhi, Alexandra Makarova
Odessa State Environmental University, Odessa, Ukraine

An energy approach (based on the Gell-Mann and Low adiabatic formalism) and operator perturbation theory method [1,2] are pplied to studying interaction of finite Fermi systems (atoms, nuclei) with a strong electric and laser field. Results of the computing energies and widths of DC, AC strong field Stark and multiphoton resonances for atoms (Tm, Gd, U) are presented. Some unusual spectral features are disciverred. A special interest attract the results of our computing the widths of the autoionization resonances in the Tm; their decay can be realized through two channels: Beutler-Fano, ROD ones. In a sufficiently weak DC electric field (!100 V/cm) widths of resonances of opposite parity are radically changed.

We also present the results of computing AC Stark shifts of single proton states in the nuclei ^{16}O, ^{168}Er in super intense laser field (I$\tilde{1}0^{25}$-10^{35} W/cm^2) and compared with available data [3]. New data are listed for the ^{57}Fe, ^{171}Yb nuclei. Shifts of several keV are reached at intensities of roughly 10^{34} W/cm^2 for ^{16}O, ^{57}Fe and 10^{32} W/cm^2 for heavier nuclei .

References: [1] A. Glushkov, L. Ivanov, J. Phys. B. **26,** L379 (1993); Phys. Lett. A **170**, 33 (1992); A. Glushkov, 2012 *Progr.Theor. Chem. Phys.* (Springer) **26,** 231 (2012); [2] A. Glushkov, *J. Phys.:Conf. Series***397,** 012011 (2012); **548,** 012020 (2014); 3] A. Glushkov, L.N. Ivanov, V.S. Letokhov, *Nuclear*

Quantum Optics, Preprint ISAN NAS4, ISAN, Troitsk, 1992; T. Bürvenich, J. Evers, C. Keitel, Phys. Rev.C **74,** 044601 (2006).

AN ADVANCED RELATIVISTIC ENERGY APPROACH IN ELECTRON-COLLISIONAL SPECTROSCOPY OF MULTICHARGED IONS IN PLASMAS

Vasily Buyadzhi
Odessa State Environmental University, Odessa, Ukraine

We have applied a generalized relativistic energy approach (REA) [1,2] combined with relativistic many-body perturbation theory to studying spectroscopic parameters (transition energies, oscillator strengths, collision cross-sections, collision strengths) of the few-body atomic systems (ions) in plasmas with taking into account of a shielding effect (in a Debye shielding approximation) and inter-particle correlations within many-body perturbation theory. In fact the uniform quantum energy approach is firstly used in a theory of spectra and spectral lines shape for the multicharged ions in a plasma. We have performed computing transition energies, oscillators strengths, collision cross-sections for a group of the low lying (plus Rydberg) transitions in spectra of the Li- and Be-like ions with a charge of a nucleus Z=26-42 and plasma parameters: density $n_e = 10^{22}$-10^{24}cm^{-3} and temperature T=0.5-2keV. A part of the data has been firstly presented. To test the results of calculations we have compared the obtained data for some ions with other authors' calculations (multiconfiguration Dirac-Fock method, relativistic coupled-cluster theory) and available experimental data [3].

References: [1] A. Glushkov, L.N. Ivanov, Phys. Lett. A **170**, 33 (1992); .P. Ivanova, L.N. Ivanov, L. Knight, Phys.Rev.A. **48**, 365 (1993); [2] S. Malinovskaya, A. Glushkov, O. Khetselius *et al.*, Int.J.Quant.Chem. **111**, 288 (2011); V. Buyadzhi, *et al.*, J.Phys.: Conf. Ser. **905**, 012003 (2017); V. Buyadzhi et al J.Phys.: Conf. Ser. **810**, 012047 (2017). [3] Yongqiang Li, Jianhua Wu, Yong Hou, and Jianmin Yuan, J. Phys. B. **41**, 145002 (2008); M. Das, R. Chaudhuri, S. Chattopadhyay, Phys. Rev. A. **85**, 042506 (2012).

ADVANCED COMPUTATIONAL APPROACH TO RYDBERG ATOMS IN A BLACK-BODY RADIATION FIELD

Andrey Svinarenko, Vasily Buyadzhi, Alexander Glushkov, Olga Khetselius, Pavel Zaichko
Odessa State Environmental University, Odessa, Ukraine

In this paper we present the results of computing the spectra, radiation amplitudes for the Rydberg Na, K, Rb, Cs atoms, ionization rates of states with n = 10-100 in the field of blackbody radiation (BBR). The starting master method is the combined energy approach and relativistic many-body perturbation theory with the zeroth model potential and quantum defect approximation [1-3]. There are received (a part of data is firstly obtained) data for radiation amplitudes, effective lifetimes, BBR-ionization velocities for $nS_{1/2}$, $nP_{1/2,3/2}$, $nD_{3/2,5/2}$ (n=5-100) states of the Rydberg atoms Na, K,Rb, Cs, in a wide temperature interval 0-600K. It is performed a detailed comparison of some obtained data for lifetimes and BBR-ionization rates with available data of advanced quasiclassical calculations by Beterov et al, Glukhov-Ovsiannikov, model calculation results by Kleppner et al, Theodosiou et al. It is established that despite on a good agreement between experimental and theoretical (on the basis of quasiclassical and other models) there is a serious deviation these data from the experiment for a number of Rydberg states n = 25-45, which is provided by no-accounting important exchange-polarization effects, including an effect of essentially non-Coulomb grouping of Rydberg levels, pressure continuum and others. These effects are taken into account in the presented approach.

References:

[1]. A.V. Glushkov, Adv. in the Theory of Quantum Systems in Chem. and Phys. (Springer) **26**, 231 (2012);

[2] O.Yu. Khetselius, Int. J. Quant.Chem. **109,** 3330(2009);

[3]. V. Buyadzhi, *et al.*, J.Phys.: Conf. Ser. **810**, 012047 (2017).

COMPUTING RADIATIVE SPECTRAL PARAMETERS OF MULTICHARGED IONS WITHIN RELATIVISTIC ENERGY APPROACH AND MODEL POTENTIAL METHOD

Eugeny Ternovsky, Olga Khetselius, Anna Kuznetsova, Dmitry Mironenko
Odessa State Environmental University, Odessa, Ukraine

We have applied a generalized relativistic energy approach (REA) [1-3] combined with the relativistic many-body perturbation theory [4,5] to studying spectroscopic parameters (transition energies, oscillator strengths, The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order optimized quantum defect and model potential approximations [1,2] are used for calculation of the energies and oscillator strengths in a set of the Li-like multicharged ions (Z=11-42,69,70). The key feature of the presented approach is an implementation of the relativistic quantum defect approximation and relativistic model potential approach into the frames of the energy approach. It should be reminded that the experimental data on the oscillator strengths for many (especially, high-Z) Li-like ions are absent. The important features of the approach used are using the optimized one-particle representation and account for the polarization effect. It should be noted that an estimate of the gauge-non-invariant contributions (the difference between the oscillator strengths values calculated with using the transition operator in the form of “length” and “velocity”) is about 0.3%, i.e. the results , obtained with using the different photon propagator gauges (the Coulomb, Babushkin, Landau gauges) are practically equal. It is self-understood that the quantum defect approximation oscillator strengths data become more exact with the growth of the principal quantum number.

References:

[1] A. Glushkov, Adv. in the Theory of Quantum Systems in Chem. and Phys. (Springer) **26**, 231 (2012); [2] O.Yu. Khetselius, Int. J. Quant.Chem. **109,** 3330(2009).

RELATIVISTIC COMPUTING EXCITED AND AUTOIONIZING STATES SPECTROSCOPIC PARAMETERS FOR SOME MULTICHARGED IONS

Eugeny Ternovsky, Andrey Svinarenko, Tatyana Tkach, Valentin Ternovsky
Odessa State Environmental University, Odessa, Ukraine

The paper is devoted to application of the a relativistic many-body PT with the Dirac-Kohn-Sham (DKS) zeroth approximation combined with the generalized energy approach to studying the single and double –excited and autoionization states in spectra of multicharged ions, in particular, spectra of He-l. Li-ike ions ($n_1 l_1 n_2 l_2$; n_1,n_2=1-10; l_1,l_2=0-3), and searching unusual futures in behaviour of these states AR in an DC electric field. The wave function zeroth basis is found from the Dirac equation with potential, which includes the optimized DKS potential, the electric potential of a nucleus. All correlation corrections of the second order and dominated classes of the higher orders diagrams (electrons screening, particle-hole interaction, mass operator iterations) are taken into account within the Green’s function method. As an example, we list the energies (Ry) of some (1s4s,4p) for the He-like krypton (KrXXXV): NIST data and theoretical (this work) data by the relativistic many-body PT with the Dirac-Kohn-Sham (DKS) zeroth approximation It carried out the detailed comparison of the obtained results with available experimental (compilation) by NIST and other theoretical data. Difference between all available data is analyzed from the viewpoint of completeness of the accounting relativistic and correlation corrections.

Universal quantum critical at finite temperature for two-dimensional disordered and clean dimerized spin-1/2 anitferromagents

Deng-Ruei Tan, Fu-Jiun Jiang
Department of Physics, National Taiwan Normal University, Taipei, Taiwan

The quantum critical regime (QCR) of a two-dimensional (2D) disordered and a 2D clean dimerized spin-1/2 Heisenberg models are studied using the first principles nonperturbative quantum Monte Carlo simulations (QMC). In particular, the three well-known universal coefficients associated with QCR are investigated in detail. While in our investigation we find the obtained results are consistent with the related analytic predictions, non-negligible finite temperature T effects are observed as well. Such an influence from T on the properties of the considered spin systems related to QCR has not been explored thoroughly before. Moreover, the most striking finding in our study is that the numerical value for one of the universal coefficients we determine is likely to be different significantly from the corresponding result(s) established in the literature. To better understand the sources for the discrepancy observed here, apart from carrying out the associated analytic calculations not considered previously, it will be desirable as well to conduct a comprehensive examination of the exotic features of QCR for other disordered and clean spin systems than those investigated in this study.

10 Soft matter and Biological Physics

Molecular modeling of polymer-grafted carbon nanotubes interacting with lipid membranes

Hwankyu Lee
Dankook University, Yongin-si, Korea, Republic of

We have performed coarse-grained molecular dynamics simulations of the self-assembly of the mixture of single-walled carbon nanotubes (SWNTs) and different types of lipids, and the interactions between SWNTs and other molecules such as lipids, polyethylene glycols (PEGs), and lipid bilayers. The following topics will be presented: (1) effects of lipid structure and PEGylation on the self-assembly of lipids and SWNTs ; (2) interparticle dispersion, membrane curvature and penetration induced by SWNTs wrapped with lipids and PEGylated lipids ; (3) membrane penetration and curvature induced by SWNTs: the effect of diameter, length, and concentration ; (4) the effect of PEG size and grafting density on the conformational transition of PEGylated SWNTs between brush and mushroom. This work aids in the rational design of the size and grafting density of PEG chains to increase the drug-delivery efficiency for applications in nanomedicine.

Monte Carlo simulation of transformation of vesicle induced by internal particles

Hibiki Itoga[1], Ryota Morikawa[1], Tsuyoshi Ueta[2], Takeshi Miyakawa[1], Yuno Natsume[3], Masako Takasu[1]
[1]Tokyo University of Pharmacy and Life Sciences, Tokyo, Japan. [2]Jikei University, Tokyo, Japan. [3]Japan Women's University, Tokyo, Japan

Shape of vesicle containing colloidal particles transforms into a pearl-necklace shape when the number of these particles and the excess area of the vesicular membrane becomes large. The mechanism of the transformation is not clear. In order to explain the experimental phenomena, we constructed two vesicle models with soft-core particles in: (i) rigid spherical shell and (ii) closed triangulated lattice. Metropolis Monte Carlo simulation for these two models were performed with changing some parameters such as the number of particles N_p and the exponent n of repulsive potential among the internal particles. We investigated the distribution and diffusion of particles and stiffness of the membrane, and showed the phase diagram of the shape of a vesicle for (N_p,n). The results revealed the influence of contained particles to the membrane. Especially we found that Dumbbell shape similar to one of pearl-necklace shape (twin shape) is caused by the network of long-range repulsion among particles.

Quantum chemical analysis of reaction indices and reaction path for drug molecules

Takao Otsuka, Noriaki Okimoto, Hiroaki Saito, Makoto Taiji
RIKEN, Osaka, Japan

In this study we report a quantum chemical study on evaluating a reactivity for drug molecules by Fukui reaction indices and minimum energy reaction paths. The Fukui indices are derived by some types

of familiar population analysis method such as Mulliken, Löwdin, Hirschfeld and so on. The minimum energy reaction path is obtained by using the nudged elastic band (NEB) calculations. We apply the Fukui indices method and the NEB calculations to the drug molecular system on metabolic reaction, and analyze and evaluate the reactive site of metabolic reaction.

Molecular dynamics study on the free energy profiles of lipid translocation across binary POPC bilayer mixtures

Hiroaki Saito[1], Tetsuya Morishita[2], Taku Mizukami[3], Kenichi Nishiyama[4], Kazutomo Kawaguchi[5], Hidemi Nagao[5]
[1]RIKEN, Suita, Japan. [2]National Institute of Advanced Industrial Science and technology (AIST), Tsukuba, Japan. [3]Japan Advanced Institute of Science and Technology (JAIST), Nomi, Japan. [4]Iwate University, Morioka, Japan. [5]Kanazawa University, Kanazawa, Japan

Addition of different lipids to membrane largely changes structural and dynamical properties of the membrane, and such changes affect the functions of membrane such as signaling and molecular translocation across the membrane. Especially cholesterol makes membrane dense and changes the state to the liquid-ordered phase above around 20 mol% of cholesterol. Such membrane condensing effect also occurs by adding other lipids; ceramide, diacylglycerol and sphingomyelin. However the differences of condensing effects by these lipids and the effects on molecular translocation like lipid flip-flop are not well known yet. In this study, we thus carry out molecular dynamics simulations of binary POPC bilayers with cholesterol, ceramide, diacylglycerol and sphingomyelin and investigate the effects of these lipids on structure and dynamics of the POPC bilayer. We also evaluate the potential mean force (PMF) of lipid translocation across the binary POPC bilayer by free energy calculations and discuss the differences of condensing effects on the lipid flip-flop in the membrane.

Molecular dynamic study on solvation free energy of water and model protein

Taku Mizukami[1], Hiroaki Saito[2]
[1]JAIST, Nomi, Ishikawa, Japan. [2]RIKEN, Suita, Osaka, Japan

Water plays an important role in biology. Numerous kinds of biomolecules activate their functions in a hydrated environment, via mechanisms that are strongly influenced by interactions with water. For example, protein folding, protein structural stability, and protein function depend on the dynamics and the structure of the surrounding water. Recently we observed a large solvation free energy change with a perturbation from native structure of a soluble protein.

In this study, we focused the effect of hydration water to the model protein system constructed by simple solutes i.e. amino acids and/or ions, in the aim to evaluate the hydration effect with respect to their configurational and/or structural changes. The solvation free energies were estimated by means of the energy representation method from the trajectory data of classical molecular dynamics simulation. The free energy profiles along to the structural changes of model proteins are estimated, and the correlation between the three-dimensional profile of density water and free energy are discussed.

11 Statistical Mechanics and Complex Systems

The coevolving voter model with spin-dependent probability of rewiring

Przemyslaw Gawronski, Maria Stojkow, Dorota Zuchowska-Skiba, Krzysztof Kułkowski
AGH University of Science and Technology, Cracow, Poland

In the coevolving voter model [1,2], an agent at a node of a social network can perform two actions: either to adjust his state (spin) to the state of a linked neighbor, or to rewire the link to another actor who is in the same state as himself. The probabilities of these actions are 1-p and p, and p is the model parameter. Here we report mean field results [3] for the case where the probability p depends on the node state. The results indicate that either the system splits into two separate networks with different spins, or one of spin orientations goes extinct. As a rule, the probability of rewiring is higher for the winning population. In both cases the stationary density of active links (i.e. links between nodes in different states) vanishes. We demonstrate also that when the probability p is the same for both spins, the stationary density of active links depends on an initial state of the network. The results are discussed in terms of homophily in social contacts.

[1] F. Vazquez, V. M. Eguiluz and M. San Miguel, Phys. Rev. Lett. 100 (2008) 108702

[2] J. Toruniewska, K. Kulakowski, K. Suchecki and J. Hołyst, Phys. Rev. E 96 (2017) 042306.

[3] K. Kulakowski, M. Stojkow, D. Zuchowska-Skiba and P. Gawronski, arXiv:1804.06650.

Studying emergent symmetry at a first-order transition with a simple model

Jun Takahashi[1], Anders Sandvik[1,2]
[1]Institute of Physics, Chinese Academy of Sciences, Beijing, China. [2]Boston University, Massachusetts, USA

Emergent symmetry has attracted attention due to its possible connections with deconfined quantum criticality, where the phase boundary between a dimerized and an antiferromagnetic state is generically continuous, although the standard Ginzburg-Landau picture predicts a first-order transition.

While emergent symmetries at multicritical points have been studied in various ways, only little is known about how the emergent symmetry should remain at first-order transition points nearby [1]. For instance, a functional renormalization group study predicts that a classical system having two different O(1) symmetries would have a bicritical point with O(2) symmetry where the critical lines meet each other [2]. However, the existence and scaling properties of the emergent symmetry at the first-order transition line separating the two ordered phases is unknown.

In this study, we conduct a large-scale Monte Carlo simulation on an XY model with extended anisotropy, which eliminates the symmetry between the X-component and the Y-component for all parameter values in the Hamiltonian. We see that this model regains O(2) symmetry at a bicritical point as previously predicted [2]. Furthermore, we observe this emergent symmetry even at the first-order transition points up to some system size depending on how far the point is from the bicritical point. We discuss how the "effective emergent symmetry" can be characterized quantitatively.

[1] B. Zhao, P. Weinberg, and A. W. Sandvik, arXiv:1804.07115

[2] A. Eichhorn et. al., Phys. Rev. E 88, 042141 (2013)

Synchronization in Nonlinear Oscillators Using A SingleVariable Control: Theory and Experiment.

Abiodun Egunjobi[1,2], OLASUNKANMI OLUSOLA[3], R.T. OGUNDARE[3], E.O. ODUFUWA[3], M.O. ESAN[3], U.E. VINCENT[3]
[1]Moshood Abiola Polytechnic, Abeokuta, Nigeria. [2]Federal University of Agriculture, Abeokuta, Nigeria. [3]UNIVERSITY OF LAGOS, LAGOS, Nigeria

This paper investigates the control for synchronization of nonlinear chaotic systems via a single variable, and a linear feedback controller and adaptive controller are proposed. A theoretical approach to control design, based on Lyapunov stability theory is presented, and validated using numerical simulations and electronic experiment. Using the Lorenz systems and Sprott systems as paradigmatic oscillators, we use off-the-shelf components on breadboard to show that based on single variable controllers, two chaotic systems can evolve into synchronous behaviour when the strength of interaction is above the critical value.

2-Dimensional Frustration Modeling

E Ghorbani, ZZ Li, C Boekema
San Jose State University, San Jose CA, USA

Computational frustration modeling can be used to study systems such as spin glasses, cuprate vortex states and also social behaviors. [1] Frustration is due to competing and random interactions among spins, atoms, proteins, or in general, characters. [2]

We define frustration of each character to be proportional to the square of the relative distance between the actual and ideal (or assigned) positions. The total frustration is recorded as a function of time, as the characters move and minimize their frustration in a two-dimensional lattice. Monte Carlo simulations are used to study the frustration decrease for different number of characters and for different assigned distances. Characters assigned to regular structures such as Thomson figures show often exponential relaxation toward the figure. Characters that are assigned to random structures show regularly power behavior. For a character set, where the ideal assignments are a row (or column) unusual behavior is observed. At early times, the frustration approaches zero following an exponential law; yet after reaching nearly zero, the frustration jumps up to substantial non-zero values; later, the frustration becomes *exactly* zero and a row (or column) is formed. We are in the process of modeling the relation between frustration and energy, and will discuss potential applications for vortex structures and protein folding. Research supported by AFC and SJSU.

[1] I M Suarez, “Modeling Frustration for Physical Systems”, Master Thesis. 3295 (1990).

[2] I M Suarez *et al*, Conf Proc 2nd Woodward Conference, Springer Verlag NY 1990; Am Phys Soc Bull 35/548 (1990).

Evaluation of Bose-Einstein integral functions

Akbari Jahan
North Eastern Regional Institute of Science and Technology, Nirjuli, Itanagar, India

The study of Bose-Einstein integral functions is crucial in the fact that they arise in various numerical

calculations of different domains of physics. The significance of gamma function and Riemann zeta function in solving such integrals has been discussed and functional equations are evaluated thereby enabling the integrals of all orders to be calculated.

ADVANCED COMPUTATIONAL APPROACH TO NONLINEAR DYNAMICS OF LASER SYSTEMS WITH ELEMENTS OF A CHAOS

Valentin Ternovsky, Alexander Mashkantsev, Sergey Kirianov, Vasily Buyadzhi, Alexander Glushkov
Odessa State Environmental University, Odessa, Ukraine

The work is devoted to carrying out new approaches to the universal quantum-dynamic and chaos-geometric modelling, analysis and prediction of a chaotic dynamics of nonlinear processes quantum-generator and laser systems. The latter include a single-modal laser with an absorbing cell, a fiber laser, a semiconductor laser coupled with feedback with delay, the system of semiconductor quantum generators, combined through a general cavity. The computing code includes a set of numerical quantum-dynamic models and such non-linear analysis methods as the correlation integral approach, multi-fractal analysis, average mutual information, surrogate data, false nearest neighbours algorithms, the Lyapunov's exponents and Kolmogorov entropy approach, spectral methods and nonlinear prediction (predicted trajectories, neural network etc) algorithms [1]. We present the results of the complete numerical investigation of a chaos generation in the low- and high-attractor time dynamics of the semiconductor GaAs/GaAlAs laser system with delayed feedback (the governing parameter: feedback strength or current injection). Besides, It has been presented new model of forecasting the low-attractor time dynamics for the first time. We present the results of the complete numerical investigation of a chaos generation in the low- and high-attractor time dynamics of the erbium one-ring fibre laser. It has been numerically shown that a chaos in the EDFL is generated via intermittency by increasing the DC bias voltage and period-doubling bifurcation by reducing the frequency modulation computers.

References:

[1] .V.Glushkov et al, in: Recent Adv. in Computer Engineering, Ed. J.Balicki.(Gdansk, WSEAS Pub.). 21, 143 (2014);

ADVANCED COMPUTATIONAL APPROACH TO DIATOMIC MOLECULES IN AN ELECTROMAGNETIC FIELD: MOLECULAR POLARIZABILITIES AND CHAOS

Anna Ignatenko, **Andrey Svinarenko**, Eugeny Ternovsky, Anna Buyadzhi
Odessa State Environmental University, Odessa, Ukraine

The processes of Rayleigh and Raman vibration scattering of a light on metastable levels of the diatomic molecules (H_2, HD, D_2, Li_2, Rb_2, Cs_2, Fr_2) are studied. An advanced approach to calculation of a polarizability of the metastable molecules is presented. New numerical algorithm to calculation of the Green's electron functions is developed with accounting for a non-spherical character of a molecular field (a generalized version of Glushkov et al method [1]). Calculations of molecular polarizability, its derivative on inter-nuclear distance, depolarization degree under Rayleigh and Raman light scattering on the frequencies of the Rb, Nd lasers are carried out. Data on the polarizabilities, its derivative on inter-nuclear distance, for example, for excited triple metastable c^3P_n, states of the H_2, HD, D_2 molecules on the frequencies of the Rb (1.78eV) and Nd (1.18eV) lasers are presented and analyzed. Relativistic generalization of the approach is presented within relativistic many-body perturbation theory. We used a quantum-dynamic model for diatomic molecule in an electromagnetic field, based on the solution of the Schrödinger equation and model potential method, and a chaos theory [2], for studying polarization time series of diatomic molecules (GeO, ZrO) interacting with a linearly polarized electromagnetic field. Even though the simple procedure is used to construct the non-linear model, the predicted results for polarization time series are quite satisfactory.

References:

[1] A. Glushkov, O. Khetselius, S. Malinovskaya, Molec.Phys. **108,** 1257 (2008).

[2] A. Glushkov et al, in: Recent Adv. in Computer Engineering, Ed. J.Balicki.(Gdansk, WSEAS Pub.). 21, 143 (2014)