Condensed Matter Physics, 2021, Vol. 24, No. 3, 30101: 1–3
DOI: 10.5488/CMP.24.30101
http://www.icmp.lviv.ua/journal

CONDENSED MATTER PHYSICS

Foreword

Yuriy Kalyuzhnyi's lifetime in Science

The papers in this special issue of "Condensed Matter Physics" have been submitted with the dedication to Professor Dr. Yuriy Kalyuzhnyi on the occasion of his 70th birthday.

Professor Yuriy Kalyuzhnyi is known as one of the leading scientists in the physics of condensed matter. His work concerns different topics in physics of liquids, as well as in physical chemistry and chemical engineering. He is currently a Leading Researcher at the Department of Soft Matter Theory, Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine. He obtained his M. Sc. in Physics from the I. Franko State University of Lviv in 1973 and the Ph. D. degree in Theoretical Physics from the Odesa I. I. Mechnikov State University in 1987 under the supervision of Ihor Yukhnoskyi and Myroslav Holovko. After receiving Ph. D. he went to Prague as a postdoc at the Institute of Chemical Process Fundamentals of the Czech Academy of Sciences to work with Ivo Nezbeda on the reference interaction site model (RISM) approach for a simple model of water. Since then, integral equations in theories of fluid have become his primary topic of his entire carrier grasping gradually more and more complex systems. He visited a number of laboratories abroad and began collaborating with prominent scientists such as George Stell at the State University of New York at Stony Brook, Lesser Blum at the University of Puerto Rico, Doug Henderson and Anthony D. J. Haymet at the University of Utah, Peter T. Cummings at the University of Tennessee in Knoxvill and Vanderbilt University in Nashville, Vojko Vlachy at the University of Ljubljana, Ken A. Dill at University of California San Francisco and later at the National Institute of Health, Gerhard Kahl at the Technical University of Vienna, and others.

Dr. Yu. Kalyuzhnyi obtained his Dr. Sci. in Physics of Colloidal Systems from the Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine in 2000. Besides being Professor of Physics of Colloidal Systems (Ministry of Educ. & Sci., Ukraine) since 2009, he also served as visiting Professor at the University of Ljubljana, Slovenia in 2015, at the J. E. Purkyně University in Ústí nad Labem, Czech Republic, in 2018 and 2020, and at the Vanderbilt University, USA, in 2019.

Professor Kalyuzhnyi has published over 110 papers to date with more than 2400 citations. Here we mention only those papers for which we feel that they have a broader impact on science. Most of his papers deal with aqueous systems (water, aqueous electrolytes, polyelectrolytes), in recent years also with colloid and protein systems, and the methods of research include integral equations with various closures (PY, HNC, MSA) and the Thermodynamic Perturbation Theory. The multidensity formalism, initiated in his work with Myroslav Holovko [1] and later on developed in his work with George Stell [2], was applied in collaboration with Vojko Vlachy to analyse the properties of highly asymmetric electrolytes of spherical shape [3]. The system studied consists of large and highly charged polyions and small counterions having one or two elementary charges. Due to strong asymmetry in size, one can treat each counterion as bondable to a limited number of polyions, while each polyion can bond an arbitrary number of counterions. A generalized version of the Ornstein-Zernike equation, which involves a multiple counterion and one polyion density, together with HNC closure conditions was derived. The simplest (two-density) version of the theory yields a very good agreement with new and existing computer simulations for both thermodynamic and structural properties of these systems. This good agreement extends into the region of parameter space where the ordinary HNC approximation does not have a convergent solution. The theory has later been applied to many similar problems including treatment of directional attraction among polyions to examine the effect of dimerization on the osmotic pressure of protein solution [4]. Into this group of papers one can also include an attempt to determine the phase equilibrium in polydisperse systems by a truncatable free energy model [5].

A next important contribution in this direction is a theoretical study performed by Yuryi together with M. Holovko and V. Vlachy [6]. The authors used the AMSA (associative MSA) to derive the close form expressions for a $(n + m)$ component mixture of sticky hard spheres with $m-$components representing polyions and n components of small ions. In all the cases studied in this contribution, the AMSA reasonably well follows the Monte Carlo data for monovalent counterions. For solutions with divalent counterions, merely a qualitative agreement is achieved [6].

Application of associative integral equation approach to polymer solutions was done in collaboration with Peter Cummings [7]. It was demonstrated that the Chandler-Silbey-Ladanyi integral equation theory for site-site molecular fluids is a limiting case of the complete association of a more general two-density integral equation theory for associating fluids developed by Wertheim. By developing the polymer PY and polymer MSA, the theory was applied to describe the properties of multicomponent neutral [8] and charged [9] hard-sphere chain models, respectively.

Tventy years ago Yuryi Kalyuzhnyi joined the colleagues at the University of California at San Francisco (later State University of New York, Stony Brook) and University of Ljubljana in studies of simple models of water and aqueous solvation. In several papers in collaboration with T. Urbič, V. Vlachy, N. Southall, and K. A. Dill, he applied Wertheim's integral equation theory (IET) and thermodynamic perturbation approach (TPT) to a two-dimensional model of water [10, 11]. They studied anomalies of liquid water, hydrophobic effect and transfer of nonpolar solute into the model water. The model quite accurately reproduces the Monte Carlo results at higher temperatures, while the predictions in cold water yield only qualitative correct trends. To correct this deficiency, the orientation-dependent integral equation theory was proposed. In the study [12], the theory is improved by an explicit introduction of an orientation dependence in the integral equation, based upon expanding the two-particle angular correlation function in orthogonal basis functions. The new theory yields a considerable improvement of the predicted structure of water, compared to Monte Carlo simulations.

In the recent ten years, Prof. Kalyuzhnyi contributed toward a better understanding of stability of protein solutions. Together with V. Vlachy and K. A. Dill, he developed intuitive models of electrolyte [13] and protein solutions [14], which can explain salt specific (i.e., Hofmeister) effects in protein solutions. The model treats all the species, water, ions, and proteins explicitly albeit approximately. The calculation is based on the Wertheim's thermodynamic perturbation theory. At the same time, in collaboration with M. Kastelic, B. Hribar-Lee and K. A. Dill, he proposed a theory to study aggregation of globular proteins [15]. With few parameters and with knowledge of the cloud-point temperatures as a function of an added salt, the model gives good predictions for the properties including the liquid-liquid coexistence curves, the second virial coefficients, and others for lysozyme as well as crystalline mixtures [16]. In the next paper of this series [17], he proposed a model to control the viscosity in aqueous solutions of monoclonal antibodies (mAb). This topic was subject of the additional studies, in particular with respect

to mAb aggregation [18]. In most cases, the calculations have been supported by experiments.

For his scientific work, Yu. V. Kalyuzhnyi received several recognitions. The most important are: in 2021 the award of the National Academy of Sciences of Ukraine "For scientific achievements", in 2019 Scholarship of the Program "Lviv system of researches" by Lviv City Council, in 2019 NASU recognition "For Mentoring of Young Scientists", in 2016 "Research excellence" of Lviv City Council, in 2009 NASU "For Professional Achievements" and in 1993 ISF (G. Soros), the award recognizing an outstanding research.

At the end, we wish Yuriy, our dear colleague, co-worker, and friend, many more successful years in Science!

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