60th birthday of Myroslav Holovko

It is a pleasure to be involved in the preparation of the festschrifts honoring the 60th birthday of our good friend and colleague Professor Myroslav Holovko.

Myroslav Holovko was born in 1943 in a small village of Chernijiv located in a beautiful area close to the Ukrainian Carpathians. After graduating in 1965 from the Ivano-Frankivsk Institute of Pedagogy he became a Ph.D. student at the Physics Department of the Lviv State University under the supervision of Professor Ihor Yukhnovskii. In 1969 Yukhnovskii became the head of Lviv Department of statistical theory of condensed states at the Institute for Theoretical Physics of the Ukrainian Academy of Sciences. From its early beginning the Lviv group experienced support and strong interest from another great Ukrainian – N.N.Bogolyubov, who was at that time Director of the Institute for Theoretical Physics. Yukhnovskii's group was a fantastic place for young people to grow up as scientists. At that time the group consisted of talented, ambitious and very enthusiastic young scientists selected among the best students who graduated mainly, but not exclusively, from Lviv University. It is interesting to note that Hartmut Krienke, who celebrated his 60th birthday last July was also a member of the Yukhnovskii's group, although Krienke came to Lviv from Rostock (Eastern Germany). Thanks to the outstanding personality of Prof. Yukhnovskii, a warm and friendly atmosphere in the group was combined with exceptionally high research standards.

In 1970 Myroslav Holovko received the degree of Ph.D. and ten years later, in 1980, the degree of Doctor of Sciences. The area of his scientific interests at that time included a statistical mechanical theory of electrolyte solutions and molten salts. To study these systems Holovko successfully contributed to the development of the optimized cluster theory (OCT). The theory is represented by a cluster expansion built on the renormalized potential that follows from the solution of the mean spherical approximation (MSA) integral equation. This choice of the renormalized potential optimizes the convergence of the cluster expansion. Holovko and his coworkers have generalized the methods used in the solution of the MSA equation for a variety of important interaction potentials. These include several versions of ion-multipole models, multicomponent ion-dipole models in a neutralizing background, multicomponent sticky ion-dipole models. Unfortunately, for different reasons, not all of these works were published in regular international journals. In this issue we provide a complete reference of some of Holovko's earlier works. During Soviet times in the English translation of some of these papers, Holovko's name has been incorrectly translated as Golovko.

The OCT was utilized by Holovko to study a variety of systems and phenomena. Having explicitly taking into account the solute-solute, solute-solvent and solvent-solvent interactions it became possible to make a quantitative study of ionic solvation. Thermodynamic functions and their derivatives with respect to the temperature and pressure were studied using Padé-approximants that utilized the corresponding MSA solutions. Important advances were achieved by extending OCT within the framework of a site-site formalism. This extension makes possible detailed investigation of the effects of the molecular shape and distribution of the charge. The combination of OCT and computer simulation techniques provided us with a set of new and interesting results concerning dielectric and dynamic properties of water. Using a microscopic approach, in which all particles of the system including those belonging to the surface are treated on the same footing, a detailed investigation of the interphase structure between the surface and electrolyte solutions was carried out. An exact solution of the Schrödinger equation for a hydrogen-like atom near an impenetrable surface was obtained.

Recent Holovko's interests concern the theory of associating liquids where he proposed a multidensity version of OCT accompanied with the corresponding extension of the MSA, which became known as the associative MSA. Further extension and modification of the multidensity formalism enabled us to set up a solid basis for a systematic investigation of ionic association in electrolyte solutions. This was published in a series of the papers in which the challenging task of describing strongly associating and/or highly asymmetric electrolyte solutions was successfully addressed. Somewhat later, the theory was used to explain the anomalous temperature dependence of the capacity of the electric double layer, to investigate the electrolyte effects in intramolecular electron-transfer reactions and to study the thermodynamic and transport properties of electrolyte solutions in weakly polar solvents. Due to the fundamental character of the formalism, its applications range from dimerizing to network-forming fluids, from the fluids of chain molecules to micelle systems, and include fluids in porous media. A simple and effective model for inverse micelles was proposed and successfully used to analyze the experimental data on the effects of adding protein on the structure, percolation and thermodynamic properties of micelle solutions. The model, which is based on the competition between surface morphology and coverage, was used to study the effects of ice roughness on its coverage by hydrogen chloride molecules. It was found that in network-forming fluids the liquid-gas phase transition is located in the percolation region. In the presence of a sticky surface, the percolation threshold on the surface is achieved earlier than in the bulk. It is demonstrated that cooperative adsorption of polymer and network-forming fluids occurs in strongly diluted regions, which was verified by the experiment. The application of the integral equation technique permits to study the effects of association on the fluid electronic structure, to generate a set of new and interesting results for anisotropic fluids, as well as for fluids in porous media.

In his 60-ty Prof. M.Holovko is a head of the Theory of Solutions Department at the Institute of Condensed Matter Physics of the National Academy of Sciences of Ukraine. He is the author and coauthor of scientific books, chapters in books and encyclopedias, numerous articles in journals. In 2003 he was elected a corresponding member of the National Academy of Sciences of Ukraine.

Finally, we thank all Myroslav Holovko's colleagues who contributed to both festschrifts collected in the Journal of Molecular Liquids and Condensed Matter Physics and wish Myroslav many enjoyable and productive years with his family, for his friends, students and colleagues.

Josef Barthel
Douglas Henderson
Andrij Trokhymchuk

Main publications

1. Yukhnovskii I.R., Holovko M.F. Statistical theory of equilibrium system composed of particles with complicate electrostatic structure. Ukr. J. Phys., 1969, vol. 4, No. 7, p. 1116–1126 (in Russian).

2. Yukhnovskii I.R., Vysochanskii V.S., Holovko M.F. Radial distribution functions of ion-dipole systems. In: Physics of liquid state. 1978, vol. 6, p. 101–114 (in Russian).

3. Yukhnovskii I.R., Holovko M.F. Statistical theory of classical equilibrium systems. Kiev, Naukova Dumka, 1980 (in Russian).

4. Yukhnovskii I.R, Gruba V.D., Holovko M.F, Kessler Yu.M. Dependence of the ionic potentials of mean force on the parameters and the form of the ion-molecular interaction. Ukr. J. Phys., 1980, vol. 25, No. 10, p. 1761–1765 (in Russian).

5. Yukhnovskii I.R., Holovko M.F., Kuryliak I.I., Soviak E.M. The method of collective variables in statistical theory of inhomogeneous ion-molecular systems. Physics of molecules, 1981, vol. 10, p. 26–43 (in Russian).

6. Holovko M.F., Pizio O.A. On the static dielectric function of simple ionic systems. Dokl. Ukr. Acad. Sci. A, 1983, vol. 2, No. 1, p. 49–52 (in Russian).

7. Pizio O.A., Holovko M.F., Trokhymchuk A. Statistical theory of molten salts: Charged hard sphere system. In: Physics of Many-Body Systems, 1983, No. 3, p. 35–47 (in Russian).

8. Golovko M.F., Yukhnovskii I.R. Approaches to the many-body theory of dense ion-dipole plasma. Application to ionic solvation. – In: The Chemical Physics of Solvation, vol. A. – Elsevier, Amsterdam, 1985, Chapt. 6, p. 207–262.

9. Holovko M.F., Kuryliak I.I., Pizio O.A., Soviak E.M. Reference interactions in the statistical theory of ion-molecular systems. – In: Problems of modern statistical physics (ed. by N.N. Bogolubov), Kiev, Naukova Dumka, 1985, p. 82–96.

10. Golovko M.F., Krienke H. General virial expansions. Mol. Phys., 1989, vol. 68, No. 4. p. 967–977.

11. Holovko M.F., Kalyuzhnyi Yu.V. Analytic solution of the reference interaction site model equation for a mixture of hard spheres and symmetric rigid molecules. J. Phys.: Condens. Matter., 1989, vol. 1, p. 2891–2909.

12. Holovko M.F., Kalyuzhnyi Yu.V. Screened potentials of the site-site ion-molecular model. The mean spherical approximation. Mol. Phys., 1989, vol. 66, p. 375–396.

13. Kovalenko A.F., Soviak E.N., Golovko M.F. Electronic states of hydrogen atom near a hard wall. Phys. Stat. Sol.(b), 1989, vol. 155, p. 549–558.

14. Golovko M.F., Protsykevich I.A. Analytic solution of the mean spherical approximation for ion-dipole model in a neutralizing background. J. Stat. Phys., 1989, vol. 54, p. 707–733.

15. Lvov S.N., Umniashkin V.A., Sharygin A., Golovko M.F. The molecular statistical theory of infinite dilute solutions based on the ion-dipole model with Lennard-Jones interactions. Fluid Phase Equilibria, 1990, vol. 58, p. 283–305.

16. Kalyuzhnyi Yu.V., Holovko M.F., Nezbeda I. Analytic solution of the RISM equation for n-atomic symmetric molecules. Czech. J. Phys., 1990, vol. 40, p. 1098–1106.

17. Holovko M.F., Kalyuzhnyi Yu.V., Heinzinger K. Electrostatic and packing contributions to the structure of water and aqueous electrolyte solutions. Z.Naturforsch., 1990, vol. 45a, p. 687–694.

18. Holovko M.F., Kalyuzhnyi Yu.V. On the effects of association in the statistical theory of ionic systems. Analytic solution of the PY-MSA version of the Wertheim theory. Mol.Phys., 1991, vol. 73, p. 1145–1157.

19. Kalyuzhnyi Yu.V., Holovko M.F., Haymet A.D.J. Integral equation theory for associating liquids: Weakly associated 2–2 electrolytes. J. Chem. Phys., 1991, vol. 95, p. 9151–9164.

20. Kovalenko A.F., Soviak E.M., Holovko M.F. On the quantum properties of adsorbed particles within the model of a hydrogen atom near a hard wall. Intern. J. Quantum Chem., 1992, vol. 42, p. 321–337.

21. Kovalenko A.F., Holovko M.F. A hydrogen-like atom near a potential barrier. J. Phys. B, 1992, vol. 25, p. L233–236.

22. Trokhymchuk A., Holovko M.F., Spohr E., Heinzinger K. Combination of computer simulation methods and optimized cluster theory in determining equilibrium properties of electrolyte solutions. Mol. Phys., 1992, vol. 77, p. 903–920.

23. Pizio O.A., Holovko M.F., Haymet A.D.J., Henderson D. On the application of the theory of inhomogeneous system for the triplet and higher-order distribution functions. J. Mol. Liq., 1993, vol. 58, p. 101–115.

24. Trokhymchuk A., Holovko M.F., Heinzinger K. Static dielectric properties of the flexible model of water. J. Chem. Phys., 1993, vol. 99, p. 2964–2971.

25. Holovko M.F., Badiali J.P. Effect of an association potential on the percolation. Application to reverse micelles containing proteins. Chem. Phys. Lett., 1993, vol. 204, p. 511–516.

26. Kalyuzhnyi Yu.V., Protsykevytch I.A., Holovko M.F. Solution of the associative Percus-Yevick approximation for n-component mixture of dimerizing hard spheres. Chem. Phys. Lett., 1993, vol. 215, p. 1–4.

27. Holovko M.F., Kovalenko A.F., Soviak E. Particle quantum properties next to non-metallic surfaces. Condens. Matter Phys. , 1993, iss. 1, p. 13–25 (in Ukrainian).

28. Badiali J.P., Russier V., Holovko M.F. Analysis of the Henderson-Abraham-Barker equation in the case of a polar liquid near a neutral hard wall. J. Chem. Phys., 1993, vol. 99, No. 10, p. 8051–8055.

29. Trokhymchuk A., Holovko M.F., Henderson D. The contribution of dipole alignment into the force between macroions in ion-dipole fluid. Mol. Phys., 1993, vol. 80, p. 1009–1020.

30. Kalyuzhnyi Yu.V., Holovko M.F. An analytical study of the effects of association in the 2–2 electrolyte solution. I. Associative mean spherical approximation. Mol. Phys., 1993, vol. 80, No. 5, p. 1165–1176.

31. Kalyuzhnyi Yu.V., Stell G., Llano-Restrepo M.L., Chapman W.G., Holovko M.F. Primitive models of chemical association: Theory and simulation for dimerization. J. Chem. Phys., 1994, vol. 101, No. 9, p. 7939–7952.

32. Kalyuzhnyi Yu.V., Vlachy V., Holovko M.F., Stell G. Multidensity integral equation theory for highly asymmetric electrolyte solutions. J. Chem. Phys., 1995, vol. 102, No. 14, p. 5770–5780.

33. Holovko M.F., Vakarin E.V. An associative version of the Henderson-Abraham-Barker equation. Mol. Phys., 1995, vol. 84, p. 1057–1064.

34. Kalyuzhnyi Yu.V., Stell G., Holovko M.F. Analytical solution of the multidensity OZ equation for polymerizing fluid. Chem. Phys. Lett., 1995, vol. 235, p. 355–364.

35. Trokhymchuk A., Holovko M.F., Heinzinger K. On the structure factor for water at small wavenumbers. Z. Naturforsch., 1995, vol. 50, p. 18–20.

36. Holovko M.F., Soviak E.M. Reference interactions in the statistical theory of electrolyte solutions. Condens. Matter Phys., 1995, iss. 6, p. 49–78.

37. Trokhymchuk A., Holovko M.F., Heinzinger K. Density and charge correlations in water. Mol. Phys., 1995, vol. 86, p. 797–808.

38. Protsykevich I.A., Duda Yu., Holovko M.F. Solution of the associative PYA for multicomponent mixture of dimerizing hard spheres with surface adhesion. Chem. Phys. Lett., 1996, vol. 248, p. 57–62.

39. Duda Yu., Kalyuzhnyi Yu.V., Holovko M.F. Solution of the associate MSA for the shielded sticky point electrolyte model. J. Chem. Phys., 1996, vol. 104, p. 1081–1089.

40. Trokhymchuk A., Pizio O., Holovko M.F., Sokolovski S. Adsorption of fluids in disordered porous media from the multidensity integral equation theory. Associative analogue of the Madden-Glandt Ornstein-Zernike approximation. J. Phys. Chem., 1996, vol. 100, p. 17004–17010.

41. Trokhymchuk A., Holovko M.F. Frequency- and wave-vector-dependent susceptibility of water. J. Phys. Chem., 1996, vol. 100, No. 2, p. 1411–1414.

42. Holovko M.F., Vakarin E.V. Density profiles of a hard-sphere chain fluid near a hard wall. Application to the adsorption onto a crystalline surface. Mol. Phys., 1996, vol. 87, No. 6, p. 1375–1394.

43. Holovko M.F., Vakarin E.V. The role of association effects in theory of an electrified interface. Mol. Phys., 1996, vol. 87, No. 1, p. 123–127.

44. Blum L., Holovko M.F., Protsykevych I.A. A solution of the multiple binding mean spherical approximation for ionic mixtures. J. Stat. Phys., 1996, vol. 84, p. 191–204.

45. Sokolowska T., Holovko M.F. Analytic solution of OZ equation in the mean spherical approximation for nematic systems. Ukr. J. Phys., 1996, vol. 41, No. 10, p. 933–939.

46. Vakarin E., Duda Yu., Holovko M.F. Integral equation theory for the four bonding sites model of associating fluids. I. Structure factor and compressibility. Mol. Phys., 1997, vol. 90, No. 4, p. 611–625.

47. Vakarin E., Holovko M.F., Duda Yu. Integral equation theory for the four bonding sites model of associating fluids. II. Density profiles and adsorption onto a solid surface. Mol. Phys., 1997, vol. 91, No. 2, p. 203–214.

48. Vakarin E., Duda Yu., Holovko M.F. Continuum percolation of the four bonding site associating fluids. J. Stat. Phys., 1997, vol. 88, No. 5/6, p. 1333–1352.

49. Trokhymchuk A., Pizio O., Holovko M.F., Sokolovski S. Associative replica OZ equations and the structure of chemically reacting fluids in porous media. J. Chem. Phys., 1997, vol. 106, No. 1, p. 200–209.

50. Vakarin E., Holovko M.F. Interfacial structure of dimerizing and hard sphere chain fluids in the vicinity of a crystalline surface: effect of a cooperative adsorption. Mol. Phys., 1997, vol. 90, No. 1, p. 63–73.

51. Kalyuzhnyi Yu.V., Blum L., Holovko M.F., Protsykevych I.A. Solution of the polymer mean spherical approximation for totally flexible sticky two-point electrolyte model. J. Mol. Liq., 1997, vol. 73/74, p. 1–26.

52. Holovko M.F., Protsykevych I.A., Kalyuzhnyi Yu.V., Blum L. Primitive model for highly asymmetric electrolytes. Associative mean spherical approximation. Physica A., 1997, vol. 236, p. 85–96.

53. HCassin G., Duda Yu.Ya., Holovko M.F., Badiali J.P., Pileni M.P. Cytochrome-c in reverse micelles. Small angle X-ray scattering measurements, percolation process and critical behavior: An interpretation with an association model. J. Chem. Phys., 1997, vol. 107, No. 7, p. 2683–2693.

54. Voronov A., Luzinov I., Minko S., Sidorenko A., Vakarin E., Holovko M.F. Adsorption of polymers at two-dimensional diluted to semidiluted regime. Macromolecules, 1997, vol. 30, p. 6929–6936.

55. Duda Yu.Ya., Holovko M.F. Structure of liquid sulfur through polymer Percus-Yevick theory. Phys. Chem. Liquid., 1997, vol. 35, p. 175–189.

56. Duda Yu., Vakarin E., Kalyuzhnyi Yu., Holovko M.F. Analytical treatment of the fused hard-sphere chain model: $0.5 < L < 1$. Physica A, 1997, vol. 245, p. 393–410.

57. Vakarin E., Duda Yu., Holovko M.F. Cooperative adsorption of network forming fluids onto crystalline surfaces. Structure and connectivity of the interface. J. Chem. Phys., 1997, vol. 107, No 14, p. 4961–4973.

58. Holovko M.F. New aspects in the theory of aqueous electrolyte solutions: the effects of cation hydrolysis and polynuclear ion formation. Condens. Matter Phys., 1997, iss. 12, p. 13–25.

59. Vakarin E., Duda Yu., Holovko M.F. Polymers near a solid surface: fused hard sphere chain model. J. Mol. Liq., 1998, vol. 75, p. 77–95.

60. Segura C.J., Vakarin E.V., Chapman W.G., Holovko M.F. A comparison of density functional and integral equation theories as Monte Carlo simulations for hard sphere associating fluids near a hard wall. J. Chem. Phys., 1998, vol. 108, No. 12, p. 4837–4848.

61. Duda Yu., Segura C.J., Vakarin E., Holovko M.F., Chapman W.G. Network forming fluids: Integral equations and Monte Carlo simulations. J. Chem. Phys., 1998, vol. 108, No. 21, p. 9168–9176.

62. Lomba E., Lopez-Martin J.L., Holovko M.F. Chemical association and electronic structure: A new theoretical approach. J. Chem. Phys., 1998, vol. 108, No. 24, p. 10175–10180.

63. Holovko M.F. The multidensity integral equation approach in the theory of complex liquids. Condens. Matter Phys., 1999, No. 2(18), p. 205–220.

64. Holovko M.F., Polishchuk Z.V. The screening potentials of ion-dipole system adsorbed in ion-dipolar disordered matrices. Condens. Matter Phys., 1999, No. 2(18), p. 267–272.

65. Holovko M.F., Sokolovska T.G. Analytical solution of the Ornstein-Zernike equation with the mean spherical closure for a nematic phase. J. Mol. Liq., 1999, vol. 82, p. 161–181.

66. Vakarin E.V., Filippov A.E., Badiali J.P., Holovko M.F. Structural rearrangement of solid surfaces due to competing adsorbate-substrate interactions. Phys. Rev. E., 1999, vol. 60, p. 660–674.

67. Holovko M.F., Vakarin E.V. Modelling of the elementary surface processes occurring in the course of heterogeneous catalytic reactions. Condens. Matter Phys., 2000, vol. 3, No. 2(22), p. 417–436.

68. Barthel J., Krienke H., Holovko M.F., Kapko V.I., Protsykevich I.A. The application of the associative mean spherical approximation in the theory of non-aqueous electrolyte solutions. Condens. Matter Phys., 2000, vol. 3, No. 3(23), p. 657–674.

69. Holovko M.F., Kapko V.I. Associative mean spherical approximation for ion-molecular systems: Ion-dipole model with ionic, molecular and ion-molecular associations. J. Mol. Liq., 2000, vol. 87, p. 109–128.

70. Holovko M.F., Kalyuzhnyi Yu.V., Druchok M.Yu. On the theory of cation hydrolysis in aqueous electrolyte solutions. J. Phys. Studies., 2000, vol. 4, No. 1, p. 100–107.

71. Sokolovska T.G., Sokolovskii R.O., Holovko M.F. Orientational ordering in fluids with partially constrained molecule orientations. Phys. Rev. E., 2000, vol. 62, p. 6771–6779.

72. Kalyuzhnyi Yu.V., Holovko M.F., Vlachy V. Highly asymmetric electrolytes in the associative mean-spherical approximation. J. Stat. Phys., 2000, vol. 100, p. 243–263.

73. Krienke H., Barthel J., Holovko M.F., Protsykevich I., Kalyuzhnyi Yu. Osmotic and activity coefficients associated electrolytes over large concentration ranges from chemical model calculations. J. Mol. Liq., 2000, vol. 87, p. 191–216.

74. Protsykevich I.A., Holovko M.F., Kondrat S.V. The reference system for a highly asymmetric electrolyte solutions: The analytical treatment. J. Mol. Liq., 2000, vol. 88, p. 65–75.

75. Holovko M.F., Sovyak E.M. Renormalized potential of nonuniform system: Ion-molecular mixture – porous media. J. Phys. Studies, 2000, vol. 4, p. 391–402.

76. Patsagan T., Trokhymchuk A., Holovko M.F. The structure and dynamical properties of the simple fluids in porous media. J. Mol. Liq., 2001, vol. 92, No. 1–2, p. 117–124.

77. Holovko M.F., Kapko V., Henderson D., Boda D. On the influence of ionic association on the capacitance of an electrical double layer. Chem. Phys. Lett., 2001, vol. 342, p. 363–368.

78. Holovko M.F., Kondrat S.V. Connection of Landau-Ginzburg models with continuous microscopic approach for self-assembling systems. J. Mol. Liq., 2001, vol. 92, No. 1–2, p. 125–130.

79. Vakarin E.V., Holovko M.F., Baidali J.P. Adsorbate induced distortion of solid surfaces. Application to HCl on ice at stratospheric conditions. Condens. Matter Phys., 2001, vol. 4, p. 251–276.

80. Sokolovska T.G., Sokolovskii R.O., Holovko M.F. Nematic model in the presence of a finite disorienting field: Integral equation approach. Phys. Rev. E., 2001, p. 051710.

81. Vakarin E.V., Holovko M.F. Adsorption of HCl on ice. Effects of the surface heterogeneity. Chem. Phys. Lett., 2001, vol. 349, p. 13–18.

82. Vakarin E.V., Holovko M.F., Piotrowiak P. Ion-pairing effects in intramolecular electron transfer. Chem. Phys. Lett., 2002, vol. 363, p. 7–12.

83. Holovko M.F. Association and clusterization in liquids and solutions. A multidensity integral equation approach. J. Mol. Liq., 2002, vol. 96–97, p. 65–85.

84. Barthel J., Krienke H., Neuder R., Holovko M.F. The role of ion-aggregate formation in the calculation of physical properties of electrolyte solutions. Fluid Phase Equilibria, 2002, vol. 194–197, p. 107–122.

85. Patsahan T., Trokhymchuk A., Holovko M.F. Computer simulations of dynamical properties of methane in a model silica gel. Condens. Matter Phys., 2003, vol. 6, No. 1(33), p. 3–21.

86. Vakarin E.V., Holovko M.F. Clustering as a mechanism of enhanced adsorption. Condens. Matter Phys., 2003, vol. 6, No. 1(33), p. 119–126.