Curriculum Vitæ and list of publications

Dr. Fantoni Riccardo
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Education

1989 "Maturità" 60/60 at Liceo Scientifico Sperimentale Filippo Buonarroti in Pisa.

1989 Matriculated at the University of Pisa, Faculty of Mathematical, Physical and Natural Sciences.

1994 November 18th: "Laurea cum laude" in Physics. Title of the thesis: "Sum rules in a layered electron gas". *Supervisor:* Prof. M. P. Tosi (Scuola Normale Superiore in Pisa).

1995 Matriculated as a graduate student at the University of Illinois at Urbana-Champaign, Department of Physics.

1997 May 18th: Master degree in Physics at the University of Illinois at Urbana-Champaign. *Supervisor:* Prof. D. M. Ceperley (Department of Physics in Urbana-Champaign).

2001 Matriculated at the XVI doctorate cycle at the University of Trieste, Department of Theoretical Physics.

2004 April 6th: "Dottorato di ricerca" (Philosophical Degree) in Physics at the University of Trieste. Title of the thesis: "Classical liquids: exact results, integral equations theory, and Monte Carlo simulations" *Supervisor:* Prof. G. Pastore (Department of Theoretical Physics in Trieste).

Positions

1996 summer: Research Assistant in the Physics department at the University of Illinois at Urbana-Champaign. Coordinators David Ceperley and Richard Martin.

1997 summer: Research Assistant in the Physics department at the University of Illinois at Urbana-Champaign. Coordinators David Ceperley and Richard Martin.

1997 fall: Research Assistant in the Physics department at the University of Illinois at Urbana-Champaign. Coordinators David Ceperley and Richard Martin.

2000 Won a Ph.D. position (BAT-O IIa/2) at the Max-Planck-Institute für Plasmaphysik, Teilinstitut Greifswald, Bereich Stellaratortheorie at the 5th of January 2000 which I declined.

2000 Research Assistant (1 year) at the Department of Mathematics and Statistics, University of Limerick, Ireland in the group of S. B. G. O'Brien.

2004 April 15th: "Assegno di ricerca" (Postdoctoral Fellowship 24 months) at the Department of Chemical Physics, University "Ca' Foscari" of Venice. Title of the project: "Analysis of proteins in solutions using statistical thermodynamic techniques". Project PRIN-COFIN2003025755-044. National coordinator Prof. Amos Maritan. Local coordinator Prof. Achille Giacometti.

2006 March 17th: "Assegno di ricerca" (Postdoctoral Fellowship 24 months) at the Department of Chemical Physics, University "Ca' Foscari" of Venice. Title of the project: "Colloidal mixtures, globular proteins and liquid crystal-like phases of biopolymers". Project PRIN-COFIN2005027330. National coordinator Prof. Amos Maritan. Local coordinator Prof. Achille Giacometti.

2009 October 15th: Postdoctoral Fellowship (36 months) at the National Institute of Theoretical Physics (NITheP), Stellenbosch Institute for Advanced Study, Matieland 7602, South Africa.

2012 January 1st: Guest (until now) at S.I.S.S.A., via Bonomea 265, 34136 Trieste, Italy.

2012 January 1st: Honorary Fellow (until now) at the Department of Molecular Science and Nanosystems, University "Ca' Foscari" of Venice, Calle Larga S. Marta DD2137, I-30123 Venezia, Italy.

2015 July 17th: Habilitation to teach Mathematics and Physics (classes A049, A048, A047, A038) in Italian high-school obtained at the University of Trieste with mark 87/100. One year course with exams. "Abilitazione all' insegnamento nella scuola secondaria per la classe A049 Matematica e Fisica con punteggio 87/100".

2016 August 24th: Passed a "Concorso per l' assunzione in ruolo nell' insegnamento di Matematica (classe A026) nella scuola secondaria di secondo grado con punteggio 72.2/100".

2017 September 1st: "Contratto a tempo indeterminato per l' insegnamento di Matematica nella scuola secondaria di secondo grado (confirmed on 1st September 2019)".

2019 May 10th: Habilitation for Associate Professor in Theoretical Physics of Matter (sector 02/B2) in the Italian University (until 10 May 2028).

Short visits and scientific collaborations

1995-2000 Collaboration in the Physics Department at the University of Illinois at Urbana-Champaign, USA with the research group of Prof. David Ceperley and Prof. Richard Martin.

2000-2001 Collaboration with the Research group of Prof. S. B. G. O'Brien at the Department of Mathematics and Statistics, University of Limerick, Ireland.

2001-2004 Collaboration with the research group of Prof. Giorgio Pastore at the Theoretical Physics Department of the University of Trieste, Italy.

2003 January: Visiting Scientist (1 month) at the University of Paris-Sud at Orsay. Scientific collaboration with the research group of Prof. Bernard Jancovici at the Laboratory of Theoretical Physics of the University of Paris-Sud at Orsay, France. Support from ECOS Nord/COLCIENCIAS-ICFES-ICETEX action C00P02 of French and Colombian cooperation. Support from COLCIENCIAS and BID through project #1204-05-10078.

2004-2006 Title of the project: "Analysis of proteins in solutions using statistical thermodynamic techniques". Project PRIN-COFIN2003025755-044. University "Ca' Foscari" of Venice, Italy. National coordinator Prof. Amos Maritan. Local coordinator Prof. Achille Giacometti.

2006-2008 Title of the project: "Colloidal mixtures, globular proteins and liquid crystal-like phases of biopolymers". Project PRIN-COFIN2005027330. University "Ca' Foscari" of Venice, Italy. National coordinator Prof. Amos Maritan. Local coordinator Prof. Achille Giacometti.

2008 Collaboration with Prof. Andres Santos supported by the Ministerio de Educación y Ciencia Spain through Grant No. FIS2007–60977. Support from the Italian MIUR (PRIN-COFIN).

2008 Collaboration with Prof. Gabriel Tellez supported by the Italian MIUR (PRIN-COFIN 2006/2007)

2009 Collaboration with the research group of Prof. Andres Santos supported by the Italian MIUR through a Grant No. PRIN-COFIN 2007B57EAB 2008/2009. Supported by the Ministry of Education, Youth, and Sports of the Czech Republic, under Project No. LC512 Center for Biomolecules and Complex Molecular Systems. Supported by the Ministerio de Educación y Ciencia Spain through Grant No. FIS2007-60977 partially financed by FEDER funds and by the Junta de Extremadura through Grant No. GRU09038.

2009 Collaboration with Prof. Andres Santos supported by the Ministerio de Educación y Ciencia Spain through Grant No. FIS2007-60977 partially financed by FEDER funds and by the Junta de Extremadura through Grant No. GRU09038. Supported by the Italian MIUR through a grant PRIN-COFIN Contract No. 2007B57EAB 2008/2009.

2009 Research group of Prof. Michael Kastner at the National Institute of Theoretical Physics of the University of Stellenbosch, South Africa.

2009-2011 Research group of Prof. K. K. Müller-Nedebock in the Physics Department at the University of Stellenbosch, South Africa.

2010 October 10th: Visiting scientist (three months) at the University of Extremadura in Badajoz, Spain. Scientific collaboration with the research group of Prof. Andrés Santos in the Physics Department at the University of Extremadura in Badajoz, Spain. Support of the PRIN-COFIN under Grant No. 2007B58EAB. Supported by the Spanish government through Grant No. FIS2007-60977, partially financed by FEDER funds. Support of the MSMT of the Czech Republic under Project No. LC512 and the GAAS of the Czech Republic Grant No. IAA400720710.

2010 Collaboration with Prof. Francesco Sciortino. Support of a PRIN-COFIN 2007B58EAB grant. Support from ERC-226207-PATCHYCOLLOIDS and ITN-234810-COMPLOIDS.

2011 Collaboration with the research group of Prof. Andres Santos. Support of PRIN-COFIN 2007B58EAB, FEDER FIS2010-16587, and GAAS IAA400720710.

2011 Collaboration with Prof. Andres Santos supported by the Ministerio de Ciencia e Innovacion (Spain) through Grant No. FIS2010-16587 and the Junta de Extremadura (Spain) through Grant No. GR10158, partially financed by FEDER funds.

2011 Research group of Prof. Bert Klumperman in the Polymer Physics Department at the University of Stellenbosch, South Africa. Support by the South African Research Chairs Initiative of the Department of Science and Technology and National Research Foundation.

2013 October 20th: Visiting Scientist (one month) at the University of Extremadura in Badajoz, Spain. Scientific collaboration with the research group of Prof. Andrés Santos in the Physics Department at the University of Extremadura in Badajoz, Spain. Supported by the Spanish government through Grant No. FIS2010-16587 and by the Junta de Extremadura (Spain) through Grant No. GR101583, partially financed by FEDER funds. Support by PRIN-COFIN 2010-2011 (Contract No. 2010LKE4CC).

2013 Collaboration with Prof. Andres Santos. Support from the Ministerio de Ciencia e Innovacion (Spain) through Grant No. FIS2010-16587 and the Junta de Extremadura. (Spain) through Grant No. GR10158, partially financed by Fondo Europeo de Desarrollo Regional (FEDER) funds.

2014 Research group of Prof. Saverio Moroni in Scuola Internazionale Superiore di Studi Avanzati (SISSA), Italy.

2014 June 15th: Visiting Scientist (one week) at the "Laboratoire de Physique ENS de Lyon", France. Scientific collaboration with the research group of Prof. Angel Alastuey.

2015 Collaboration with Prof. Giorgio Pastore. Support by PRIN-COFIN 2010–2011 (contract 2010LKE4CC).

2015 Collaboration with Prof. Andres Santos. Support from PRIN-MIUR 2010-2011 project (Contract No. 2010LKE4CC). Supported by the Spanish Government through Grant No. FIS2013-42840-P and by the Regional Government of Extremadura (Spain) through Grant No. GR15104 (partially financed by ERDF funds).

2017 January 8th: Visiting Scientist (two months) at the University of Extremadura in Badajoz, Spain. Scientific collaboration with the research group of Prof. Andrés Santos in the Physics Department at the University of Extremadura in Badajoz, Spain. Support of the Ministerio de Economía y Competitividad (Spain) through Grant No. FIS2016-76359-P and the Junta de Extremadura (Spain) through Grant No. GR15104, both partially financed by "Fondo Europeo de Desarrollo Regional" funds.

2018 March 26th: Visiting Scientist (one week) at the "Laboratoire de Physique ENS de Lyon", France. Scientific collaboration with the research group of Prof. Angel Alastuey.

2021 Collaboration with the research group of Prof. Andres Santos. Support from Grant PID2020-112936GB-I00 funded by MCIN/AEI/10.13039/501100011033, and from Grants

IB20079 and GR18079 funded by Junta de Extremadura (Spain) and by ERDF A way of making Europe.

Research Interests

Non-Equilibrium Statistical Mechanics:	From the Liouvillian dynamics to the Fokker-Planck equation. From the Fokker-Planck equation to the Smoluchowski equation. The Langevin equation. Monte Carlo solution of the Smoluchowski equation.
Statistical Mechanics:	Sum rules in many body systems, many body models soluble exactly analytically, integral equation theories for fluids (Percus-Yevick, hypernetted chain, mean spherical approximation, rational function approximation,...), thermodynamic perturbation theories, Monte Carlo methods, stochastic processes.
Condensed and Soft Matter Physics:	Coulomb liquids, the polaron, Bosons fluids, colloidal suspensions, polymers.
Quantum fluid models:	The Jellium in one, two, and three spatial dimensions and the polaron problem. The Jellium on parallel planes. Square-well Bosons as a model of cold atoms. The ^{4}He in three and two dimensions.
Classical fluid models:	The one-dimensional nearest-neighbor fluids, the one- and two-component plasma living in one-, two-, and three-dimensions, the one- and two-component plasma living on curved surfaces, the hard-sphere fluid, the penetrable square-well fluid in one-, two-, and three-dimensions, the non-additive hard-sphere mixture, the Widom-Rowlinson model, the sticky-hard-sphere one- and two-component fluid, the restricted primitive model for charged hard spheres, patchy spheres fluids (the Janus fluid, etc ...).
Quantum field theory	Path integral Monte Carlo of lattice field theory subject to different kinds of quantization procedures.
Numerical methods (NM) of interest:	The solution of integral equation theories and the Monte Carlo methods to perform computer experiments.
NM for the solution of integral equation theories:	The Newton Raphson algorithm (with conjugated gradient method) and the Picard algorithm.
NM for Monte Carlo simulations:	Ground state Monte Carlo simulations (variational and diffusion), path integral Monte Carlo simulations (conventional and worm algorithm), classical Monte Carlo simulations (NVT, NPT, grand canonical, Gibbs ensemble).

Abstract: Aim of the research is to develop analytical and computational methods for condensed and soft matter starting from the fundamental many-body equations. Apart from the few analytically exactly solvable models our principal instruments are Integral Equation Theory, Density Functional

Theory, Thermodynamic Perturbation Theory, Association Theory, and Monte Carlo simulations which can find exact properties of many-body systems. We are combining these approaches to create new methods and to test the accuracy of calculations on materials. Current studied materials include colloidal suspensions, ionic liquids, polymer mixtures, the electron fluid, the polaron, and boson fluids (like ^{4}He, ^{4}He-H_2 mixtures, ...). We investigate the structure and thermodynamic properties of the materials including their phase transitions like the gas-liquid-solid first order ones, the percolation threshold, the clustering, the localization, the demixing, the polydispersity, and surface properties.

Teaching at the University of Illinois in Urbana-Champaign

1995 fall: Teaching Assistant in the Physics department at the University of Illinois at Urbana-Champaign. Grading on *Electricity and Magnetism II* [physics 336], undergraduate level, lecturer J. Thaler.

1996 spring: Teaching Assistant in the Physics department at the University of Illinois at Urbana-Champaign. Grading on *Electricity and Magnetism I* [physics 335], undergraduate level, lecturer S. J. Chang.

1996 fall: Teaching Assistant in the Physics department at the University of Illinois at Urbana-Champaign. Grading on *Biomolecular Physics* [physics 450], graduate level, lecturer E. Gratton.

1997 spring: Teaching Assistant in the Physics department at the University of Illinois at Urbana-Champaign. Discussion section on *Waves in Physics* [physics 108], undergraduate level, lecturer J. Wolfe.

1998 spring: Teaching Assistant in the Physics department at the University of Illinois at Urbana-Champaign. Discussion and Laboratory sections on *Thermal Physics and Fluids* [physics 113], undergraduate level, lecturer M. B. Weissman.

1998 summer: Teaching Assistant in the Physics department at the University of Illinois at Urbana-Champaign. Discussion and Laboratory section on *Classical Mechanics* [physics 101], undergraduate level, lecturer J. Kocik.

1998 fall: Teaching Assistant in the Physics department at the University of Illinois at Urbana-Champaign. Laboratory section on *Electricity, Magnetism, and Optics* [physics 112], undergraduate level, lecturers D. Hertzog, N. Makins, and G. Gladding.

1999 spring: Teaching Assistant in the Physics department at the University of Illinois at Urbana-Champaign. Laboratory section on *Waves and Quantum mechanics/Thermal Physics and Fluids* [physics 113/114], undergraduate level, lecturers D. Beck, J. Thaler, and L. Cooper.

Teaching at the "Università Ca' Foscari di Venezia"

2004-2005 "Metodi Matematici per Scienze e Tecnologie dei Materiali", fourth year first semester, 4 Credits (32 hours), graduate level, lecturer.

2004-2005 "Istituzioni di Matematica II per Scienze e Tecnologie dei Materiali", second year second semester, 4 Credits (32 hours), graduate level, lecturer.

2005-2006 "Metodi Matematici per Scienze e Tecnologie dei Materiali", fourth year first semester, 4 Credits (32 hours), graduate level, lecturer.

Teaching at the "Università di Trieste"

2008-2009 "Fisica Generale per Ingegneria Industriale", first year second semester, 9 Credits (75 hours), graduate level, lecturer.

2012-2013 "Laboratorio di Fisica III (Ottica)", second year second semester, 7 Credits (35 hours), graduate level, assistant. Lecturer Giuseppe della Ricca.

2013-2014 "Laboratorio di Calcolo", first year second semester, 6 Credits (45 hours), graduate level, assistant. Lecturer Giorgio Pastore.

2016-2017 "Laboratorio di Calcolo", first year second semester, 6 Credits (70 hours), graduate level, assistant. Lecturer Giorgio Pastore.

Teaching in the Italian secondary school of second degree, didactic activity, seminars to students

2014-2015 Teaching at "Galileo Galilei" high school in Trieste in informatics (A042 18h) [25/10/14-26/11/14]; several seminar activities to the students.

2015 Habilitation to teach Mathematics and Physics (A049-A027) in Italian high-school ("Liceo") [17/7/15]

2015-2016 Teaching at "ITS A. Volta" high school in Trieste in mathematics and physics (A049 18h) [12/10/15-14/12/15]; Teaching at ISIS "G. Carducci" high school in Trieste in mathematics and physics (A049 13h+5h) [14/12/15-30/06/16]; several seminar activities to the students.

2016-2017 Teaching at "Francesco Petrarca" high school in Trieste in mathematics and physics (A049 8h) [26/09/16-10/10/16]; Teaching at "ITS G. Deledda-M. Fabiani" high school in Trieste in mathematics (A026 7h) [08/03/17-14/06/17]; several seminar activities to the students.

2017-2018 Won the "Concorso per l'immissione in Ruolo" to teach Mathematics (A026) in Italian high-school ("Scuola Secondaria di Secondo Grado") [24/08/16]; Teaching at "ITS Fermo Solari" high school in Tolmezzo in mathematics (A026 18h) [6/09/17-20/10/17]; several seminar activities to the students.

2018-now Teaching at "ISIS Nautico T. di Savoia - L. Galvani" high school in Trieste in mathematics (A026 18h) [10/09/18-now]; several seminar activities to the students.

Publications

I have **73 publications** with an **h-index of 15**, a total sum of the **times cited of 668**, **24** publications where I am the **only author**, and **39** publications where I am the **first author**. These data are extracted from the ISI database on September 2022. Follows the list of publications:

(1) **Fantoni R.** and Tosi M.P., Nuovo Cimento **17D**, 155 (1995)
Title: "Decay of correlations and related sum rules in a layered classical plasma"
Abstract: The asymptotic behaviours of particle correlation functions and the related sum rules are discussed for a layered classical plasma with e^2/r interactions in the fluid state, in dependence on the number of layers. These properties derive from consistency conditions imposed by screening on the hierarchical equations, as already treated by A. Alastuey and Ph.A. Martin (J. Stat. Phys., **39**, 405 (1985)) for various Coulomb fluids. The main results concern i) the type of clustering of correlations needed for the validity of multipolar sum rules at various orders, ii) the proof that the pair correlation function in a finite multilayer may carry an electric dipole moment and the calculation of its partioning among the layers, and iii) the dimensionality crossover in an infinitely extended or periodically repeated multilayer with varying interlayer spacing and wave vector.

(2) **Fantoni R.** and Tosi M.P., Nuovo Cimento **17D**, 1165 (1995)
Title: "Coordinate space form of interacting reference response function of d-dimensional jellium"
Abstract: The interacting reference response function $\chi_I^3(k)$ of three-dimensional jellium in k space was defined by Niklasson (1974) in terms of the momentum distribution of the interacting electron assembly. Here the Fourier transform $F_I^d(r)$ of $\chi_I^d(k)$ is studied for the jellium model with e^2/r interactions in dimensionality $d = 1, 2$ and 3, in an extension of recent work by Holas, March and Tosi for the case $d = 3$. The small-r and large-r forms of $F_I^d(r)$ are explicitly evaluated from the analytic behaviour of the momentum distribution $n_d(p)$. In the appendix, a model of $n_d(p)$ is constructed which interpolates between these limits.

(3) **Fantoni R.** and Tosi M.P., Physica B **217**, 35 (1996)
Title: "Some properties of short-range correlations for electrons in quantum wires"
Abstract: The asymptotic behaviours of the momentum distribution, the static structure factor and the local field factor at large momenta are evaluated for the jellium model of an interacting electron fluid confined in a quantum wire. The dependence of the results on the character of the confinement and their relevance to models of the dielectric screening function are discussed.

(4) **Fantoni R.**, Jancovici B., and Téllez G., J. Stat. Phys. **112**, 27 (2003)
Title: "Pressures for a One-Component Plasma on a Pseudosphere"
Abstract: The classical (i.e. non-quantum) equilibrium statistical mechanics of a two-dimensional one-component plasma (a system of charged point-particles embedded in a neutralizing background) living on a pseudosphere (an infinite surface of constant negative curvature) is considered. In the case of a flat space, it is known that, for a one-component plasma, there are several reasonable definitions of the pressure, and that some of them are not equivalent to each other. In the present paper, this problem is revisited in the case of a pseudosphere. General relations between the different pressures are given. At one special

temperature, the model is exactly solvable in the grand canonical ensemble. The grand potential and the one-body density are calculated in a disk, and the thermodynamic limit is investigated. The general relations between the different pressures are checked on the solvable model.

(5) **Fantoni R.** and Pastore G., J. Chem. Phys. **119**, 3810 (2003)
Title: "Generating functionals, consistency, and uniqueness in the integral equation theory of liquids"
Abstract: We discuss and illustrate through numerical examples the relations between generating functionals, thermodynamic consistency (in particular the virial-free energy one), and uniqueness of the solution, in the integral equation theory of liquids. We propose a new approach for deriving closures automatically satisfying such characteristics. Results from a first exploration of this program are presented and discussed.

(6) **Fantoni R.** and Pastore G., Phys. Rev. E **68**, 046104 (2003)
Title: "Stability of the iterative solutions of integral equations as one phase freezing criterion"
Abstract: A recently proposed connection between the threshold for the stability of the iterative solution of integral equations for the pair correlation functions of a classical fluid and the structural instability of the corresponding real fluid is carefully analyzed. Direct calculation of the Lyapunov exponent of the standard iterative solution of HNC and PY integral equations for the 1D hard rods fluid shows the same behavior observed in 3D systems. Since no phase transition is allowed in such 1D system, our analysis shows that the proposed one phase criterion, at least in this case, fails. We argue that the observed proximity between the numerical and the structural instability in 3D originates from the enhanced structure present in the fluid but, in view of the arbitrary dependence on the iteration scheme, it seems uneasy to relate the numerical stability analysis to a robust one-phase criterion for predicting a thermodynamic phase transition.

(7) **Fantoni R.** and Pastore G., Physica A **332**, 349 (2004)
Title: "Direct correlation functions of the Widom-Rowlinson model"
Abstract: We calculate, through Monte Carlo numerical simulations, the partial total and direct correlation functions of the three dimensional symmetric Widom-Rowlinson mixture. We find that the differences between the partial direct correlation functions from simulation and from the Percus-Yevick approximation (calculated analytically by Ahn and Lebowitz) are well fitted by Gaussians. We provide an analytical expression for the fit parameters as function of the density. We also present Monte Carlo simulation data for the direct correlation functions of a couple of non additive hard sphere systems to discuss the modification induced by finite like diameters.

(8) **Fantoni R.** and Pastore G., J. Chem. Phys. **120**, 10681 (2004)
Title: "Computer simulation study of the closure relations in hard sphere fluids"
Abstract: We study, using Monte Carlo simulations, the cavity and the bridge functions of various hard sphere fluids: one component system, equimolar additive and non additive binary mixtures. In particular, we numerically check the assumption of local dependency of the bridge functions from the indirect correlation functions, on which most of the existing integral equation theories hinge. We find that this condition can be violated either in the region around the first and second neighbors shell, or inside the hard core,

for the systems here considered. The violations manifest themselves clearly in the so called Duh-Haymet plots of the bridge functions versus the indirect correlation functions and become amplified as the coupling of the system increases.

(9) **Fantoni R.**, Gazzillo D., Giacometti A., J. Chem. Phys. **122**, 034901 (2005)
Title: "Stability boundaries, percolation threshold, and two phase coexistence for polydisperse fluids of adhesive colloidal particles"
Abstract: We study the polydisperse Baxter model of sticky hard spheres (SHS) in the modified Mean Spherical Approximation (mMSA). This closure is known to be the zero-order approximation (C0) of the Percus-Yevick (PY) closure in a density expansion. The simplicity of the closure allows a full analytical study of the model. In particular we study stability boundaries, the percolation threshold, and the gas-liquid coexistence curves. Various possible sub-cases of the model are treated in details. Although the detailed behavior depends upon the particularly chosen case, we find that, in general, polydispersity inhibits instabilities, increases the extent of the non percolating phase, and diminishes the size of the gas-liquid coexistence region. We also consider the first-order improvement of the mMSA (C0) closure (C1) and compare the percolation and gas-liquid boundaries for the one-component system with recent Monte Carlo simulations. Our results provide a qualitative understanding of the effect of polydispersity on SHS models and are expected to shed new light on the applicability of SHS models for colloidal mixtures.

(10) **Fantoni R.**, Gazzillo D., Giacometti A., Phys. Rev. E **72**, 011503 (2005)
Title: "The thermodynamic instabilities of a binary mixture of sticky hard spheres"
Abstract: The thermodynamic instabilities of a binary mixture of sticky hard spheres (SHS) in the modified Mean Spherical Approximation (mMSA) and the Percus-Yevick (PY) approximation are investigated using an approach devised by X. S. Chen and F. Forstmann [J. Chem. Phys. 97, 3696 (1992)]. This scheme hinges on a diagonalization of the matrix of second functional derivatives of the grand canonical potential with respect to the particle density fluctuations. The zeroes of the smallest eigenvalue and the direction of the relative eigenvector characterize the instability uniquely. We explicitly compute three different classes of examples. For a symmetrical binary mixture, analytical calculations, both for mMSA and for PY, predict that when the strength of adhesiveness between like particles is smaller than the one between unlike particles, only a pure condensation spinodal exists; in the opposite regime, a pure demixing spinodal appears at high densities. We then compare the mMSA and PY results for a mixture where like particles interact as hard spheres (HS) and unlike particles as SHS, and for a mixture of HS in a SHS fluid. In these cases, even though the mMSA and PY spinodals are quantitatively and qualitatively very different from each other, we prove that they have the same kind of instabilities. Finally, we study the mMSA solution for five different mixtures obtained by setting the stickiness parameters equal to five different functions of the hard sphere diameters. We find that four of the five mixtures exhibit very different type of instabilities. Our results are expected to provide a further step toward a more thoughtful application of SHS models to colloidal fluids.

(11) **Fantoni R.**, Gazzillo D., Giacometti A., and Sollich P. J. Chem. Phys. **125**, 164504 (2006)
Title:"Phase behavior of weakly polydisperse sticky hard spheres: Perturbation theory for the Percus-Yevick solution"

Abstract: We study the effects of size polydispersity on the gas-liquid phase behavior of mixtures of sticky hard spheres. To achieve this, the system of coupled quadratic equations for the contact values of the partial cavity functions of the Percus-Yevick solution [R. J. Baxter, J. Chem. Phys. **49**, 2770 (1968)] is solved within a perturbation expansion in the polydispersity, i.e., the normalized width of the size distribution. This allows us to make predictions for various thermodynamic quantities which can be tested against numerical simulations and experiments. In particular, we determine the leading order effects of size polydispersity on the cloud curve delimiting the region of two-phase coexistence and on the associated shadow curve; we also study the extent of size fractionation between the coexisting phases. Different choices for the size dependence of the adhesion strengths are examined carefully; the Asakura-Oosawa model [J. Chem. Phys. **22**, 1255 (1954)] of a mixture of polydisperse colloids and small polymers is studied as a specific example.

(12) Gazzillo D., Giacometti A., **Fantoni R.**, and Sollich P., Phys. Rev. E. **74**, 051407 (2006)
Title: "Multicomponent adhesive hard sphere models and short-ranged attractive interactions in colloidal or micellar solutions"
Abstract: We investigate the dependence of the stickiness parameters $t_{ij} = 1/(12\tau_{ij})$ where the τ_{ij} are the conventional Baxter parameters on the solute diameters σ_i and σ_j in multicomponent sticky hard sphere (SHS) models for fluid mixtures of mesoscopic neutral particles. A variety of simple but realistic interaction potentials, utilized in the literature to model short-ranged attractions present in real solutions of colloids or reverse micelles, is reviewed. We consider: (i) van der Waals attractions, (ii) hard-sphere-depletion forces, (iii) polymer-coated colloids, and (iv) solvation effects (in particular hydrophobic bonding and attractions between reverse micelles of water-in-oil microemulsions). We map each of these potentials onto an equivalent SHS model by requiring the equality of the second virial coefficients. The main finding is that, for most of the potentials considered, the size-dependence of $t_{ij}(T, \sigma_i, \sigma_j)$ can be approximated by essentially the same expression, i.e., a simple polynomial in the variable $\sigma_i\sigma_j/\sigma_{ij}^2$, with coefficients depending on the temperature T, or for depletion interactions on the packing fraction η_0 of the depletant particles.

(13) Gazzillo D., **Fantoni R.**, and Giacometti A., Mol. Phys. **104**, 3451 (2006)
Title: "Phase behavior of polydisperse sticky hard spheres: analytical solutions and perturbation theory"
Abstract: We discuss phase coexistence of polydisperse colloidal suspensions in the presence of adhesion forces. The combined effect of polydispersity and Baxter's sticky-hard-sphere (SHS) potential, describing hard spheres interacting via strong and very short-ranged attractive forces, give rise, within the Percus-Yevick (PY) approximation, to a system of coupled quadratic equations which, in general, cannot be solved either analytically or numerically. We review and compare two recent alternative proposals, which we have attempted to by-pass this difficulty. In the first one, truncating the density expansion of the direct correlation functions, we have considered approximations simpler than the PY one. These C_n approximations can be systematically improved. We have been able to provide a complete analytical description of polydisperse SHS fluids by using the simplest two orders C_0 and C_1, respectively. Such a simplification comes at the price of a lower accuracy in the phase diagram, but has the advantage of providing an analytical description of various new phenomena associated with the onset of polydispersity in phase equilibria (e.g. fractionation). The second approach is based on a perturbative expansion

of the polydisperse PY solution around its monodisperse counterpart. This approach provides a sound approximation to the real phase behavior, at the cost of considering only weak polydispersity. Although a final settlement on the soundness of the latter method would require numerical simulations for the polydisperse Baxter model, we argue that this approach is expected to keep correctly into account the effects of polydispersity, at least qualitatively.

(14) **Fantoni R.**, Gazzillo D., Giacometti A., Miller M. A., and Pastore G., J. Chem. Phys. **127**, 234507 (2007)
Title: "Patchy sticky hard spheres: analytical study and Monte Carlo simulations"
Abstract: We consider a fluid of hard spheres bearing one or two uniform circular adhesive patches, distributed so as not to overlap. Two spheres interact via a "sticky" Baxter potential if the line joining the centers of the two spheres intersects a patch on each sphere, and via a hard sphere potential otherwise. We analyze the location of the fluid-fluid transition and of the percolation line as a function of the size of the patch (the fractional coverage of the sphere's surface) and of the number of patches within a virial expansion up to third order and within the first two terms (C0 and C1) of a class of closures Cn hinging on a density expansion of the direct correlation function. We find that the locations of the two lines depend sensitively on both the total adhesive coverage and its distribution. The treatment is almost fully analytical within the chosen approximate theory. We test our findings by means of specialized Monte Carlo (MC) simulations and find the main qualitative features of the critical behaviour to be well captured in spite of the low density perturbative nature of the closure. The introduction of anisotropy is a first step towards a more realistic model of globular proteins in solution.

(15) Gazzillo D., **Fantoni R.**, and Giacometti A., Phys. Rev. E **78**, 021201 (2008)
Title: "Fluids of spherical molecules with dipolarlike nonuniform adhesion: an analytically solvable anisotropic model"
Abstract: We consider an anisotropic version of Baxter's model of 'sticky hard spheres', where a nonuniform adhesion is implemented by adding, to an isotropic surface attraction, an appropriate 'dipolar sticky' correction (positive or negative, depending on the mutual orientation of the molecules). The resulting nonuniform adhesion varies continuously, in such a way that in each molecule one hemisphere is 'stickier' than the other. We derive a complete analytic solution by extending a formalism [M. S. Wertheim, J. Chem. Phys. **55**, 4281 (1971)] devised for dipolar hard spheres. Unlike Wertheim's solution which refers to the 'mean spherical approximation', we employ a *Percus-Yevick closure with orientational linearization*, which is expected to be more reliable. We obtain analytic expressions for the orientation-dependent pair correlation function $g(1,2)$. Only one equation for a parameter K has to be solved numerically. We also provide very accurate expressions which reproduce K as well as some parameters, Λ_1 and Λ_2, of the required Baxter factor correlation functions with a relative error smaller than 1%. We give a physical interpretation of the effects of the anisotropic adhesion on the $g(1,2)$. The model could be useful for understanding structural ordering in complex fluids within a unified picture.

(16) Santos A., **Fantoni R.**, and Giacometti A., Phys. Rev. E **77**, 051206 (2008)
Title: "Penetrable square-well fluids: Exact results in one dimension."
Abstract: We introduce a model of attractive penetrable spheres by adding a short-range

attractive square well outside a penetrable core, and we provide a detailed analysis of structural and thermodynamical properties in one dimension using the exact impenetrable counterpart as a starting point. The model is expected to describe star polymers in regimes of good and moderate solvent under dilute conditions. We derive the exact coefficients of a low-density expansion up to second order for the radial distribution function and up to fourth order in the virial expansion. These exact results are used as a benchmark to test the reliability of approximate theories (Percus-Yevick and hypernetted chain). Notwithstanding the lack of an exact solution for arbitrary densities, our results are expected to be rather precise within a wide range of temperatures and densities. A detailed analysis of some limiting cases is carried out. In particular, we provide a complete solution of the sticky penetrable-sphere model in one dimension up to the same order in density. The issue of Ruelle' s thermodynamics stability is analyzed and the region of a well-defined thermodynamic limit is identified.

Appears in the SklogWiki:
`http://www.sklogwiki.org/SklogWiki/index.php/Penetrable_square_well_model`

(17) **Fantoni R.** and Téllez G., J. Stat. Phys. **133**, 449 (2008)
Title: "Two-dimensional one-component plasma on a Flamm' s paraboloid"
Abstract: We study the classical non-relativistic two-dimensional one-component plasma at Coulomb coupling $\Gamma = 2$ on the Riemannian surface known as Flamm' s paraboloid which is obtained from the spatial part of the Schwarzschild metric. At this special value of the coupling constant, the statistical mechanics of the system is exactly solvable analytically. The Helmholtz free energy asymptotic expansion for the large system has been found. The density of the plasma, in the thermodynamic limit, has been carefully studied in various situations.

(18) **Fantoni R.**, Giacometti A., Malijevský A., and Santos A., J. Chem. Phys. **131**, 124106 (2009)
Title: "Penetrable-Square-Well fluids: Analytical study and Monte Carlo simulations"
Abstract: We study structural and thermophysical properties of a one-dimensional classical fluid made of penetrable spheres interacting via an attractive square-well potential. Penetrability of the spheres is enforced by reducing from infinite to finite the repulsive energy barrier in the pair potentials As a consequence, an exact analytical solution is lacking even in one dimension. Building upon previous exact analytical work in the low-density limit [Santos *et al.*, Phys. Rev. E **77**, 051206 (2008)], we propose an approximate theory valid at any density and in the low-penetrable regime. By comparison with specialized Monte Carlo simulations and integral equation theories, we assess the regime of validity of the theory. We investigate the degree of inconsistency among the various routes to thermodynamics and explore the possibility of a fluid-fluid transition. Finally we locate the dependence of the Fisher-Widom line on the degree of penetrability. Our results constitute the first systematic study of penetrable spheres with attractions as a prototype model for soft systems.

Appears in the SklogWiki:
`http://www.sklogwiki.org/SklogWiki/index.php/Penetrable_square_well_model`

(19) Gazzillo D., **Fantoni R.**, and Giacometti A., Phys Rev. E **80**, 061207 (2009)
Title: "Local orientational ordering in fluids of spherical molecules with dipolar-like

anisotropic adhesion."
Abstract: We discuss some interesting physical features stemming from our previous analytical study of a simple model of a fluid with dipolar-like interactions of very short range in addition to the usual isotropic Baxter potential for adhesive spheres. While the isotropic part is found to rule the global structural and thermodynamical equilibrium properties of the fluid, the weaker anisotropic part gives rise to an interesting short-range local ordering into a periodically modulated structure with preferred antiparallel alignment.

(20) Santos A., **Fantoni R.**, and Giacometti A., J. Chem. Phys. **131**, 181105 (2009)
Title: "Thermodynamic consistency of energy and virial routes: An exact proof within the linearized Debye-Hückel theory"
Abstract: The linearized Debye-Hückel theory for liquid state is shown to provide thermodynamically consistent virial and energy routes for any potential and for any dimensionality. The importance of this result for bounded potentials is discussed.

Has been among the 14th most downloaded JCP articles in the month of November.

(21) **Fantoni R.**, Giacometti A., Malijevský A., and Santos A., J. Chem. Phys. **133**, 024101 (2010)
Title: "A numerical test of a high-penetrability approximation for the one-dimensional penetrable-square-well model"
Abstract: The one-dimensional penetrable-square-well fluid is studied using both analytical tools and specialized Monte Carlo simulations. The model consists of a penetrable core characterized by a finite repulsive energy combined with a short-range attractive well. This is a many-body one-dimensional problem, lacking an exact analytical solution, for which the usual van Hove theorem on the absence of phase transition does not apply. We determine a high-penetrability approximation complementing a similar low-penetrability approximation presented in previous work. This is shown to be equivalent to the usual Debye-Hückel theory for simple charged fluids for which the virial and energy routes are identical. The internal thermodynamic consistency with the compressibility route and the validity of the approximation in describing the radial distribution function is assessed by a comparison against numerical simulations. The Fisher-Widom line separating the oscillatory and monotonic large-distance behaviors of the radial distribution function is computed within the high-penetrability approximation and compared with the opposite regime, thus providing a strong indication of the location of the line in all possible regimes. The high-penetrability approximation predicts the existence of a critical point and a spinodal line, but this occurs outside the applicability domain of the theory. We investigate the possibility of a fluid-fluid transition by the Gibbs ensemble Monte Carlo techniques, not finding any evidence of such a transition. Additional analytical arguments are given to support this claim. Finally, we find a clustering transition when Ruelle's stability criterion is not fulfilled. The consequences of these findings on the three-dimensional phase diagrams are also discussed.

(22) **Fantoni R.**, J. Stat. Mech. P07030 (2010)
Title: "Non existence of a phase transition for the Penetrable Square Well model in one dimension"
Abstract: Penetrable Square Wells in one dimension were introduced for the first time in [A. Santos *et. al.*, Phys. Rev. E, **77**, 051206 (2008)] as a paradigm for ultra-soft colloids.

Using the Kastner, Schreiber, and Schnetz theorem [M. Kastner, Rev. Mod. Phys., **80**, 167 (2008)] we give strong evidence for the absence of any phase transition for this model. The argument can be generalized to a large class of model fluids and complements the van Hove's theorem.

(23) **Fantoni R.**, A. Giacometti, F. Sciortino, and G. Pastore, Soft Matter **7**, 2419 (2011)
Title: "Cluster theory of Janus particles"
Abstract: We apply a simple statistical mechanics cluster approximation for studying clustering in the Kern and Frenkel model of Janus fluids. The approach is motivated by recent Monte Carlo simulations work on the same model revealing that the vapor coexisting with the liquid phase contains clusters of different sizes and shapes whose equilibrium concentrations in general depend on the interaction range as well as on thermodynamic parameters. The approximation hinges on a separation between the intra- and inter-cluster interactions, where the former are explicitly computed by Monte Carlo simulations. Two simple liquid theory approximations are exploited for the description of the latter. In the first we use the ideal-gas expressions and obtain a qualitative agreement with extensive Monte Carlo bulk simulations. This can be improved to a semi-quantitative agreement, by using a hard-sphere description for the cluster-cluster interaction.

Has been the 5th most read article in Soft Matter on the month of February:
`http://blogs.rsc.org/sm/2011/03/28/`
Appeared as a hot article in the Soft Matter Blog in the month of February:
`http://blogs.rsc.org/sm/2011/02/`

(24) **Fantoni R.**, A. Malijevský, A. Santos, and A. Giacometti, Europhys. Lett. **93**, 26002 (2011)
Title: "Phase diagram of the penetrable square well-model"
Abstract: We study a system formed by soft colloidal spheres attracting each other via a square-well potential, using extensive Monte Carlo simulations of various nature. The softness is implemented through a reduction of the infinite part of the repulsive potential to a finite one. For sufficiently low values of the penetrability parameter we find the system to be Ruelle stable with square-well like behavior. For high values of the penetrability the system is thermodynamically unstable and collapses into an isolated blob formed by a few clusters each containing many overlapping particles. For intermediate values of the penetrability the system has a rich phase diagram with a partial lack of thermodynamic consistency.

Appears in the SklogWiki:
`http://www.sklogwiki.org/SklogWiki/index.php/Penetrable_square_well_model`

(25) **Fantoni R.**, A. Malijevský, A. Santos, and A. Giacometti, Mol. Phys. **109**, 2723 (2011)
Title: "The penetrable square-well model: extensive versus non-extensive phases"
Abstract: The phase diagram of the penetrable square-well fluid is investigated through Monte Carlo simulations of various nature. This model was proposed as the simplest possibility of combining bounded repulsions at short scale and short-range attractions. We prove that the model is thermodynamically stable for sufficiently low values of the penetrability parameter, and in this case the system behaves similarly to the square-well model. For larger penetration, there exists an intermediate region where the system is metastable, with well defined fluid-fluid and fluid-solid transitions, at finite size, but

eventually becomes unstable in the thermodynamic limit. We characterize the unstable non-extensive phase appearing at high penetrability, where the system collapses into an isolated blob of a few clusters of many ovelapping particles each.

Appears in the SklogWiki:
`http://www.sklogwiki.org/SklogWiki/index.php/Penetrable_square_well_model`

(26) **Fantoni R.** and K. K. Müller-Nedebock, Phys. Rev. E **84**, 011808 (2011)
Title: "Field-theoretical approach to a dense polymer with an ideal binary mixture of clustering centers"
Abstract: We propose a field-theoretical approach to a polymer system immersed in an ideal mixture of clustering centers. The system contains several species of these clustering centers with different functionality, each of which connects a fixed number segments of the chain to each other. The field theory is solved using the saddle point approximation and evaluated for dense polymer melts using the Random Phase Approximation. We find a short-ranged effective inter-segment interaction with strength dependent on the the average segment density and discuss the structure factor within this approximation. We also determine the fractions of linkers of the different functionalities.

(27) **Fantoni R.** and Santos A., Phys. Rev. E **84**, 041201 (2011)
Title: "Nonadditive hard-sphere fuid mixtures. A simple analytical theory"
Abstract: We construct a non-perturbative fully analytical approximation for the thermodynamics and the structure of non-additive hard-sphere fluid mixtures. The method essentially lies in a heuristic extension of the Percus-Yevick solution for additive hard spheres. Extensive comparison with Monte Carlo simulation data shows a generally good agreement, especially in the case of like-like radial distribution functions.

(28) **Fantoni R.**, Eur. Phys. J. B **85**, 108 (2012)
Title: "A cluster theory for a Janus fluid"
Abstract: Recent Monte Carlo simulations on the Kern and Frenkel model of a Janus fluid have revealed that in the vapor phase there is the formation of preferred clusters made up of a well-defined number of particles: the micelles and the vesicles. A cluster theory is developed to approximate the exact clustering properties stemming from the simulations. It is shown that the theory is able to reproduce the micellisation phenomenon.

(29) **Fantoni R.**, J. Stat. Mech. P04015 (2012)
Title: "Two Component Plasma in a Flamm's Paraboloid"
Abstract: The two component plasma (TCP) living in a Flamm's paraboloid is studied at a value of the coupling constant $\Gamma = 2$ for which an analytic expression for the grand canonical partition function is available. Two cases are considered, the plasma in the half surface with an insulating horizon and the plasma in the whole surface. The Green's function equation necessary to determine the n-particle truncated correlation functions is explicitly found. In both cases this proves too complicated to be solved analytically. So we present the method of solution reducing the problem to finding the two linearly independent solutions of a linear homogeneous second order ordinary differential equation with polynomial coefficients of high degrees. In the flat limit one recovers the solution for the structure of the TCP in a plane in the first case but the collapse of opposite charges at the horizon makes the structure of the plasma physically not well defined in the second case.

(30) **Fantoni R.**, Salari J. W. O., Klumperman B., Phys. Rev. E **85**, 061404 (2012)
Title: "The structure of colloidosomes with tunable particle density: simulation *vs* experiment"
Abstract: Colloidosomes are created in the laboratory from a Pickering emulsion of water droplets in oil. The colloidosomes have approximately the same diameter and by choosing (hairy) particles of different diameters it is possible to control the particle density on the droplets. The experiment is performed at room temperature. The radial distribution function of the assembly of (primary) particles on the water droplet is measured in the laboratory and in a computer experiment of a fluid model of particles with pairwise interactions on the surface of a sphere.

(31) **Fantoni R.**, Phys. Rev. B **86**, 144304 (2012)
Title: "Localization of acoustic polarons at low temperatures: A path integral Monte Carlo approach"
Abstract: We calculate the low temperature properties of an acoustic polaron in three dimensions in thermal equilibrium at a given temperature using a specialized path integral Monte Carlo method. In particular we show that the chosen Hamiltonian for the acoustic polaron describes a phase transition from a localized state to an unlocalized state for the electron as the phonon-electron coupling constant decreases. The phase transition manifests itself with an jump discontinuity in the potential energy as a function of the coupling constant. In the weak coupling regime the electron is in an extended state whereas in the strong coupling regime it is found in the self-trapped state.

(32) **Fantoni R.**, J. Stat. Mech. P10024 (2012)
Title: "The density of a fluid on a curved surface"
Abstract: We discuss the property of the number density of a fluid of particles living in a curved surface without boundaries to be constant in the thermodynamic limit. In particular we find a sufficient condition for the density to be constant along the Killing vector field generating a given isometry of the surface and the relevant necessary condition. We then show that the Coulomb fluid on any open surface asymptotically flat with a conformal metric with a conformal factor not a function of the azimuthal angle must have constant density in the thermodynamic limit.

(33) **Fantoni R.**, Physica B **412**, 112 (2013)
Title: "Low temperature acoustic polaron localization"
Abstract: We calculate the properties of an acoustic polaron in three dimensions in thermal equilibrium at a given low temperature using the path integral Monte Carlo method. The specialized numerical method used is described in full details, thus complementing our previous paper [R. Fantoni, Phys. Rev. B **86**, 144304 (2012)], and it appears to be the first time it has been used in this context. Our results are in favor of the presence of a phase transition from a localized state to an extended state for the electron as the phonon-electron coupling constant decreases. The phase transition manifests itself with a jump discontinuity in the potential energy as a function of the coupling constant and it affects the properties of the path of the electron in imaginary time: In the weak coupling regime the electron is in an extended state whereas in the strong coupling regime it is found in a self-trapped state.

(34) **Fantoni R.**, Solid State Communications **159**, 106 (2013)
Title: "Hellmann and Feynman theorem versus diffusion Monte Carlo experiment"

Abstract: We discuss about the importance, in a computer experiment, of the choice of suitable estimators to measure a physical quantity. In particular we propose a new direct route to determine estimators for observables which do not commute with the Hamiltonian, which make use of the Hellmann and Feynman theorem. In a diffusion Monte Carlo simulation this introduces a new bias to the measure due to the choice of the auxiliary function which is independent from the bias due to the choice of the trial wave function. We used this route to measure the radial distribution function of a spin one half Fermion fluid.

(35) **Fantoni R.** and Pastore G., Europhys. Lett., **101**, 46003 (2013)
Title: "The restricted primitive model of ionic fluids with nonadditive diamaters"
Abstract: The restricted primitive model with nonadditive hard-sphere diameters is shown to have interesting and peculiar clustering properties. We report accurate calculations of the cluster concentrations. Implementing efficient and ad hoc Monte Carlo algorithms we determine the effect of nonadditivity on both the clustering and the gas-liquid binodal. For negative nonadditivity, tending to the extreme case of completely overlapping unlike ions, the prevailing clusters are made of an even number of particles having zero total charge. For positive nonadditivity, the frustrated tendency to segregation of like particles and the reduced space available to the ions favors percolating clusters at high densities.

(36) Maestre M. A. G., **Fantoni R.**, Giacometti A. and Santos A., J. Chem. Phys. **138**, 094904 (2013)
Title: "Janus fluid with fixed patch orientations: theory and simulations"
Abstract: We study thermophysical properties of a Janus fluid with constrained orientations, using analytical techniques and numerical simulations. The Janus character is modeled by means of a Kern-Frenkel potential where each sphere has one hemisphere of square-well and the other of hard-sphere character. The orientational constraint is enforced by assuming that each hemisphere can only point either North or South with equal probability. The analytical approach hinges on a mapping of the above Janus fluid onto a binary mixture interacting via a "quasi" isotropic potential. The anisotropic nature of the original Kern-Frenkel potential is reflected by the asymmetry in the interactions occurring between the unlike components of the mixture. A rational-function approximation extending the corresponding symmetric case is obtained in the sticky limit, where the square-well becomes infinitely narrow and deep, and allows a fully analytical approach. Notwithstanding the rather drastic approximations in the analytical theory, this is shown to provide a rather precise estimate of the structural and thermodynamical properties of the original Janus fluid.

(37) **Fantoni R.** and Santos A., Phys. Rev. E **87**, 042102 (2013)
Title: "Multicomponent fluid of nonadditive hard spheres near a wall"
Abstract: A recently proposed rational-function approximation [Phys. Rev. E **84**, 041201 (2011)] for the structural properties of nonadditive hard spheres is applied to evaluate analytically (in Laplace space) the local density profiles of multicomponent nonadditive hard-sphere mixtures near a planar nonadditive hard wall. The theory is assessed by comparison with NVT Monte Carlo simulations of binary mixtures with a size ratio $1:3$ in three possible scenarios: a mixture with either positive or negative nonadditivity near an additive wall, an additive mixture with a nonadditive wall, and a nonadditive mixture with a nonadditive wall. It is observed that, while the theory tends to underestimate

the local densities at contact (especially in the case of the big spheres) it captures very well the initial decay of the densities with increasing separation from the wall and the subsequent oscillations.

(38) **Fantoni R.** and Pastore G., Phys. Rev. E **87**, 052303 (2013)
Title: "Monte Carlo simulation of the nonadditive restricted primitive model of ionic fluids: Phase diagram and clustering"
Abstract: We report an accurate Monte Carlo calculation of the phase diagram and clustering properties of the restricted primitive model with non-additive hard-sphere diameters. At high density the positively non-additive fluid shows more clustering than the additive model and the negatively non-additive fluid shows less clustering than the additive model, at low density the reverse scenario appears. A negative nonadditivity tends to favor the formation of neutrally charged clusters starting from the dipole. A positive nonadditivity favors the pairing of like ions at high density. The critical point of the gas-liquid phase transition moves at higher temperatures and higher densities for a negative nonadditivity and at lower temperatures and lower densities for a positive nonadditivity. The law of corresponding states does not seem to hold strictly. Our results can be used to interpret recent experimental works on room temperature ionic liquids.

Appeared on the Kaleidoscope of PRE on the month of May:
`http://pre.aps.org/kaleidoscope/pre/87/5/052303`

(39) **Fantoni R.**, Eur. Phys. J. B **86**, 286 (2013)
Title: "Radial distribution function in a diffusion Monte Carlo simulation of a Fermion fluid between the ideal gas and the Jellium model"
Abstract: We study, through the diffusion Monte Carlo method, a spin one-half fermion fluid, in the three dimensional Euclidean space, at zero temperature. The point particles, immersed in a uniform "neutralizing" background, interact with a pair-potential which can be continuously changed from zero to the Coulomb potential depending on a parameter μ. We determine the radial distribution functions of the system for various values of density, μ, and polarization. We discuss about the importance, in a computer experiment, of the choice of suitable estimators to measure a physical quantity. The radial distribution function is determined through the usual histogram estimator and through an estimator determined via the use of the Hellmann and Feynman theorem. In a diffusion Monte Carlo simulation the latter route introduces a new bias to the measure of the radial distribution function due to the choice of the auxiliary function. This bias is independent from the usual one due to the choice of the trial wave function. A brief account of the results from this study were presented in a recent communication [R. Fantoni, Solid State Communications, **159**, 106 (2013)].

(40) **Fantoni R.**, Giacometti A., Maestre M. A. G., and Santos A., J. Chem. Phys. **139**, 174902 (2013)
Title: "Phase diagrams of Janus fluids with up-down constrained orientations"
Abstract: A class of binary mixtures of Janus fluids formed by colloidal spheres with the hydrophobic hemispheres constrained to point either up or down are studied by means of Gibbs ensemble Monte Carlo simulations and simple analytical approximations. These fluids can be experimentally realized by the application of an external static electrical field. The gas-liquid and demixing phase transitions in five specific models with different patch-patch affinities are analyzed. It is found that a gas-liquid transition is present in

all the models, even if only one of the four possible patch-patch interactions is attractive. Moreover, provided the attraction between like particles is stronger than between unlike particles, the system demixes into two subsystems with different composition at sufficiently low temperatures and high densities.

(41) **Fantoni R.** and Santos A., J. Chem. Phys. **140**, 244513 (2014)
Title: "Depletion force in the infinite-dilution limit in a solvent of nonadditive hard spheres"
Abstract: The mutual entropic depletion force felt by two solute "big" hard spheres immersed in a binary mixture solvent of nonadditive "small" hard spheres is calculated as a function of the surface-to-surface distance by means of canonical Monte Carlo simulations and through a recently proposed rational-function approximation [Phys. Rev. E **84**, 041201 (2011)]. Four representative scenarios are investigated: symmetric solute particles and the limit where one of the two solute spheres becomes a planar hard wall, in both cases with symmetric and asymmetric solvents. In all cases, the influence on the depletion force due to the nonadditivity in the solvent is determined in the mixed state. Comparison between results from the theoretical approximation and from the simulation shows a good agreement for surface-to-surface distances greater than the smallest solvent diameter.

(42) **Fantoni R.** and Pastore G., J. Chem. Phys **141**, 074108 (2014)
Title: "Wertheim and Bjerrum-Tani-Henderson theories for associating fluids: a critical assessment"
Abstract: Two theories for associating fluids recently used to study clustering in models for self-assembling patchy particles, Wertheim's and Bjerrum-Tani-Henderson theories, are carefully compared. We show that, for a fluid allowing only for dimerization, Wertheim theory is equivalent to the Bjerrum-Tani-Henderson theory neglecting intercluster correlations. Nonetheless, while the former theory is able to account for percolation and condensation, the latter is not. For the Bjerrum-Tani-Henderson theory we also rigorously prove the uniqueness of the solution for the cluster's concentrations and the reduction of the system of equations to a single one for a single unknown. We carry out Monte Carlo simulations of two simple models of dimerizing fluids and compare quantitatively the predictions of the two theories with the simulation data.

(43) **Fantoni R.**, Phys. Rev. E **90**, 020102(R) (2014)
Title: "Gas-liquid coexistence for the bosons square-well fluid and the ^{4}He binodal anomaly"
Abstract: The binodal of a boson square-well fluid is determined as a function of the particle mass through the newly devised quantum Gibbs ensemble Monte Carlo algorithm [R. Fantoni and S. Moroni, *to be published*]. In the infinite mass limit we recover the classical result. As the particle mass decreases the gas-liquid critical point moves at lower temperatures. We explicitely study the case of a quantum delocalization de Boer parameter close to the one of ^{4}He. For comparison we also determine the gas-liquid coexistence curve of ^{4}He for which we are able to observe the binodal anomaly below the λ-transition temperature.

(44) **Fantoni R.** and Moroni S., J. Chem. Phys. **141**, 114110 (2014)
Title: "Quantum Gibbs ensemble Monte Carlo"
Abstract: We present a path integral Monte Carlo method which is the full quantum analogue of the Gibbs ensemble Monte Carlo method of Panagiotopoulos to study the gas-liquid coexistence line of a classical fluid. Unlike previous extensions of Gibbs ensemble

Monte Carlo to include quantum effects, our scheme is viable even for systems with strong quantum delocalization in the degenerate regime of temperature. This is demonstrated by an illustrative application to the gas-superfluid transition of ^{4}He in two dimensions.

(45) **Fantoni R.** and Pastore G., Mol. Phys. **113**, 2593 (2015)
Title: "Wertheim perturbation theory: thermodynamics and structure of patchy colloids"
Abstract: We critically discuss the application of the Wertheim's theory to classes of complex associating fluids that can be today engineered in the laboratory as patchy colloids and to the prediction of their peculiar gas-liquid phase diagrams. Our systematic study, stemming from perturbative version of the theory, allows us to show that, even at the simplest level of approximation for the inter-cluster correlations, the theory is still able to provide a consistent and stable picture of the behavior of interesting models of self-assembling colloidal suspension. We extend the analysis of a few cases of patchy systems recently introduced in the literature. In particular, we discuss for the first time in detail the consistency of the structural description underlying the perturbative approach and we are able to prove a consistency relationship between the valence as obtained from thermodynamics and from the structure for the one-site case. A simple analytical expression for the structure factor is proposed.

(46) **Fantoni R.**, Giacometti A., and Santos A., J. Chem. Phys. **142**, 224905 (2015)
Title: "Bridging and depletion mechanisms in colloid-colloid effective interactions: A reentrant phase diagram?"
Abstract: A general class of nonadditive sticky-hard-sphere binary mixtures, where small and large spheres represent the solvent and the solute, respectively, is introduced. The solute-solute and solvent-solvent interactions are of hard-sphere type, while the solute-solvent interactions are of sticky-hard-sphere type with tunable degrees of size nonadditivity and stickiness. Two particular and complementary limits are studied using analytical and semi-analytical tools. The first case is characterized by zero nonadditivity, lending itself to a Percus–Yevick approximate solution from which the impact of stickiness on the spinodal curves and on the effective solute-solute potential is analyzed. In the opposite nonadditive case, the solvent-solvent diameter is zero and the model can then be reckoned as an extension of the well-known Asakura–Oosawa model with additional sticky solute-solvent interaction. This latter model has the property that its exact effective one-component problem involves only solute-solute pair potentials for size ratios such that a solvent particle fits inside the interstitial region of three touching solutes. In particular, we explicitly identify the three competing physical mechanisms (depletion, pulling, and bridging) giving rise to the effective interaction. Some remarks on the phase diagram of these two complementary models are also addressed through the use of the Noro–Frenkel criterion and a first-order perturbation analysis. Our findings suggest reentrance of the fluid-fluid instability as solvent density (in the first model) or adhesion (in the second model) is varied. Some perspectives in terms of the interpretation of recent experimental studies of microgels adsorbed onto large polystyrene particles are discussed.

(47) **Fantoni R.**, Phys. Rev. E **92**, 012133 (2015)
Title: "Two phase coexistence for the hydrogen-helium mixture"
Abstract: We use our newly constructed quantum Gibbs ensemble Monte Carlo algorithm to perform computer experiments for the two phase coexistence of a hydrogen-helium mixture. Our results are in quantitative agreement with the experimental results of C.

M. Sneed, W. B. Streett, R. E. Sonntag, and G. J. Van Wylen. The difference between our results and the experimental ones is in all cases less than 15% relative to the experiment, reducing to less than 5% in the low helium concentration phase. At the gravitational inversion between the vapor and the liquid phase, at low temperatures and high pressures, the quantum effects become relevant. At extremely low temperature and pressure the first component to show superfluidity is the helium in the vapor phase.

(48) **Fantoni R.**, Eur. Phys. J. B **89**, 1 (2016)
Title: "Supercooled superfluids in Monte Carlo simulations"
Abstract: We perform path integral Monte Carlo simulations to study the imaginary time dynamics of metastable supercooled superfluid states and nearly superglassy states of a one component fluid of spinless bosons square wells. Our study shows that the identity of the particles and the exchange symmetry is crucial for the frustration necessary to obtain metastable states in the quantum regime. Whereas the simulation time has to be chosen to determine whether we are in a metastable state or not, the imaginary time dynamics tells us if we are or not close to an arrested glassy state.

(49) Alastuey A. and **Fantoni R.**, J. Stat. Phys. **163**, 887 (2016)
Title: "Fourth moment sum rule for the charge correlations of a two-component classical plasma"
Abstract: We consider an ionic fluid made with two species of mobile particles carrying either a positive or a negative charge. We derive a sum rule for the fourth moment of equilibrium charge correlations. Our method relies on the study of the system response to the potential created by a weak external charge distribution with slow spatial variations. The induced particle densities, and the resulting induced charge density, are then computed within density functional theory, where the free energy is expanded in powers of the density gradients. The comparison with the predictions of linear response theory provides a thermodynamical expression for the fourth moment of charge correlations, which involves the isothermal compressibility as well as suitably defined partial compressibilities. The familiar Stillinger-Lovett condition is also recovered as a by-product of our method, suggesting that the fourth moment sum rule should hold in any conducting phase. This is explicitly checked in the low density regime, within the Abe-Meeron diagrammatical expansions. Beyond its own interest, the fourth-moment sum rule should be useful for both analyzing and understanding recently observed behaviours near the ionic critical point.

(50) **Fantoni R.**, Physica A **457**, 406 (2016)
Title: "The Square-Shoulder-Asakura-Oosawa model"
Abstract: A new model for a colloidal size-asymmetric binary mixture is proposed: The Square-Shoulder-Asakura-Oosawa. This belongs to the larger class of non-additive hard-spheres models and has the property that its effective pair formulation is exact whenever the solvent particle fits inside the interstitial region of three touching solute particles. Therefore one can study its properties from the equivalent one-component effective problem. Some remarks on the phase diagram of this new model are also addressed.

(51) **Fantoni R.**, J. Stat. Phys. **163**, 1247 (2016)
Title: "Exact results for one dimensional fluids through functional integration"
Abstract: We review some of the exactly solvable one dimensional continuum fluid models

of equilibrium classical statistical mechanics under the unified setting of functional integration in one dimension. We make some further developments and remarks concerning fluids with penetrable particles. We then apply our developments to the study of the Gaussian core model for which we are unable to find a well defined thermodynamics.

(52) **Fantoni R.**, J. Stat. Phys. **166**, 1334 (2017)
Title: "One-dimensional fluids with positive potentials"
Abstract: We study a class of one-dimensional classical fluids with penetrable particles interacting through positive, purely repulsive, pair-potentials. Starting from some lower bounds to the total potential energy, we draw results on the thermodynamic limit of the given model.

(53) **Fantoni R.**, Physica A **477C**, 187 (2017)
Title: "The moment sum-rules for ionic liquids at criticality"
Abstract: We discuss the first three well known moment charge-charge sum-rules for a general ionic liquid. For the special symmetric case of the Restricted Primitive Model, Das, Kim, and Fisher (2011) has recently discovered, through Monte Carlo simulations, that the Stillinger-Lovett or second-moment sum-rule fails at criticality. We critically discuss a possible explanation for this unexpected behavior. On the other hand the fourth-moment sum-rule turns out to be able to account for the results of the simulations at criticality.

(54) **Fantoni R.**, J. Stat. Phys. **168**, 652 (2017)
Title: "Andersen-Weeks-Chandler perturbation theory and one-component sticky-hard-spher"
Abstract: We apply second order Andersen-Weeks-Chandler perturbation theory to the one-component sticky-hard-spheres fluid. We compare the results with the mean spherical approximation, the Percus-Yevick approximation, two generalized Percus-Yevick approximations, and the Monte Carlo simulations.

(55) **Fantoni R.** and Santos A., J. Stat. Phys. **169**, 1171 (2017)
Title: "One-Dimensional Fluids with Second Nearest-Neighbor Interactions"
Abstract: As is well known, one-dimensional systems with interactions restricted to first nearest neighbors admit a full analytically exact statistical-mechanical solution. This is essentially due to the fact that the knowledge of the first nearest-neighbor probability distribution function, $p_1(r)$, is enough to determine the structural and thermodynamic properties of the system. On the other hand, if the interaction between second nearest-neighbor particles is turned on, the analytically exact solution is lost. Not only the knowledge of $p_1(r)$ is not sufficient anymore, but even its determination becomes a complex many-body problem. In this work we systematically explore different approximate solutions for one-dimensional second nearest-neighbor fluid models. We apply those approximations to the square-well and the attractive two-step pair potentials and compare them with Monte Carlo simulations, finding an excellent agreement.

(56) **Fantoni R.**, J. Stat. Mech. P113101 (2017)
Title: "White-dwarf equation of state and structure: the effect of temperature"
Abstract: We study the effect of having a finite temperature on the equation of state and structure of a white dwarf. In order to keep the treatment as general as possible we carry out our discussion for ideal quantum gases obeying both the Fermi-Dirac and the

Bose-Einstein statistics even though we only use the results for the free electron gas inside a white dwarf. We discuss the effect of temperature on the stability of the star and on the Fermi hole.

(57) **Fantoni R.**, J. Stat. Mech. P043101 (2018)
Title: "Effect of quantum dispersion on the radial distribution function of a one-component sticky-hard-sphere fluid"
Abstract: In this short communication we present a possible scheme to study the radial distribution function of the quantum slightly polydisperse Baxter sticky hard sphere liquid at finite temperature through a semi-analytical method devised by Chandler and Wolynes.

(58) **Fantoni R.**, Int. J. Mod. Phys. C **29**, 1850028 (2018)
Title: "Two component boson-fermion plasma at finite temperature"
Abstract: We discuss thermodynamic stability of neutral real (quantum) matter from the point of view of a computer experiment at finite, nonzero, temperature. We perform (restricted) path integral Monte Carlo simulations of the two component plasma where the two species are both bosons, both fermions, and one boson and one fermion. We calculate the structure of the plasma and discuss about the formation of binded couples of oppositely charged particles. The purely bosonic case is thermodynamically unstable. In this case we find an undetermined size-dependent contact value unlike partial radial distribution function. For the purely fermionic case, we find a demixing transition with binding also of like species.

(59) **Fantoni R.**, Int. J. Mod. Phys. C **29**, 1850064 (2018)
Title: "One-component fermion plasma on a sphere at finite temperature"
Abstract: We study through a computer experiment, using the restricted path integral Monte Carlo method, a one-component fermion plasma on a sphere at finite, non-zero, temperature. We extract thermodynamic properties like the kinetic and internal energy per particle and structural properties like the radial distribution function. This study could be relevant for the characterization and better understanding of the electronic properties of hollow graphene spheres.

(60) **Fantoni R.**, Physica A **5**, 682 (2018)
Title: "From the Liouville to the Smoluchowski equation for a colloidal solute particle in a solvent"
Abstract: We show how the Smoluchowski dynamics of a colloidal Brownian particle suspended in a molecular solvent can be reached starting from the microscopic Liouvillian evolution of the full classical model in the high friction limit. The integration of the solvent degrees of freedom goes through a multiple time scale perturbation expansion which removes the secular divergences. A simple dynamical Monte Carlo scheme is then proposed to solve the resulting evolution equation for the colloid solute particle. In particular we study the approach to the equilibrium Boltzmann distribution at late times and its resilience behavior at shorter times as influenced by the steepness of the external potential and the friction coefficient around their respective minima. This is very important to understand the fate of the Brownian particle's random walk and its evolution history.

(61) **Fantoni R.**, Physica A **524**, 177 (2019)
Title: "Plasma living in a curved surface at some special temperature"

Abstract: The simplest statistical mechanics model of a Coulomb plasma in two spatial dimensions admits an exact analytic solution at some special temperature in several (curved) surfaces. We present in a unifying perspective these solutions for the (non-quantum) plasma, made of point particles carrying an absolute charge , in thermal equilibrium at a temperature $T = e^2/2k_B$, with k_B Boltzmann's constant, discussing the importance of having an exact solution, the role of the curvature of the surface, and the densities of the plasma.

(62) **Fantoni R.**, Indian J. Phys. **95**, 1027 (2021)
Title: "Form invariance of the moment sum-rules for jellium with the addition of short-range terms in the pair-potential"
Abstract: We find the first three (even) structure factor moments for a (non-quantum) one-component Jellium made of particles living in three dimensions and interacting with a Coulomb pair-potential plus a short-range term with either a finite range or decaying exponentially fast at large distances. Starting from the hierarchical Born-Green-Yvon equations we show that they are all form invariant respect to the addition of the short-range term. We discuss the relevance of the present study to interpret the failure of the moment sum-rules of ionic-liquids at criticality.

(63) **Fantoni R.**, J. Low Temp. Phys. **202**, 247 (2021)
Title: How should we choose the boundary conditions in a simulation which could detect anyons in one and two dimensions? *Abstract:* We discuss the problem of anyonic statistics in one and two spatial dimensions from the point of view of statistical physics. In particular we want to understand how the choice of the Born-von Karman or the twisted periodic boundary conditions necessary in a Monte Carlo simulation to mimic the thermodynamic limit of the many body system influences the statistical nature of the particles. The particles can either be just bosons, when the configuration space is simply connected as for example for particles on a line. They can be bosons and fermions, when the configuration space is doubly connected as for example for particles in the tridimensional space or in a Riemannian surface of genus greater or equal to one (on the torus, etc ...). They can be scalar anyons with arbitrary statistics, when the configuration space is infinitely connected as for particles on the plane or in the circle. They can be scalar anyons with fractional statistics, when the configuration space is the one of particles on a sphere. One can further have multi components anyons with fractional statistics when the configuration space is doubly connected as for particles on a Riemannian surface of genus greater or equal to one. We determine an expression for the canonical partition function of hard core particles (including anyons) on various geometries. We then show how the choice of boundary condition (periodic or open) in one and two dimensions determines which particles can exist on the considered surface.

(64) **Fantoni R.**, Eur. Phys. J. B **94**, 63 (2021)
Title: Jellium at finite temperature using the restricted worm algorithm
Abstract: We study the Jellium model of Wigner at finite, non zero, temperature through a computer simulation using the canonical path integral worm algorithm where we successfully implemented the fixed node free particles restriction necessary to circumvent the fermion sign problem. Our results show good agreement with the recent simulation data of Brown et al. and of other similar computer experiments on the Jellium model at high density and low temperature. Our algorithm can be used to treat any quantum

fluid model of fermions at finite, non zero, temperature and has never been used before in literature.

(65) **Fantoni R.** and Klauder J. R., Phys. Rev. D **103**, 076013 (2021)
Title: Affine quantization of $(\varphi^4)_4$ succeeds while canonical quantization fails
Abstract: Covariant scalar field quantization, nicknamed $(\varphi^r)_n$, where r denotes the power of the interaction term and $n = s + 1$ where s is the spatial dimension and 1 adds time. Models such that $r < 2n/(n-2)$ can be treated by canonical quantization, while models such that $r > 2n/(n-2)$ are nonrenormalizable, leading to perturbative infinities, or, if treated as a unit, emerge as 'free theories'. Models such as $r = 2n/(n-2)$, e.g., $r = n = 4$, again using canonical quantization also become 'free theories', which must be considered quantum failures. However, there exists a different approach called affine quantization that promotes a different set of classical variables to become the basic quantum operators and it offers different results, such as models for which $r > 2n/(n-2)$, which has recently correctly quantized $(\varphi^{12})_3$. In the present paper we show, with the aid of a Monte Carlo analysis, that one of the special cases where $r = 2n/(n-2)$, specifically the case $r = n = 4$, can be acceptably quantized using affine quantization.

(66) **Fantoni R.**, J. Stat. Mech. P083102 (2021)
Title: Monte Carlo evaluation of the continuum limit of $(\phi^{12})_3$
Abstract: We study canonical and affine versions of non-renormalizable euclidean classical scalar field-theory with twelfth-order power-law interactions on three dimensional lattices through the Monte Carlo method. We show that while the canonical version of the model turns out to approach a "free-theory" in the continuum limit, the affine version is perfectly well defined as an interaction model.

(67) **Fantoni R.** and Klauder J. R., J. Stat. Phys. **184**, 28 (2021)
Title: Monte Carlo evaluation of the continuum limit of the two-point function of the Euclidean free real scalar field subject to affine quantization
Abstract: We study canonical and affine versions of the quantized covariant Euclidean free real scalar field-theory on four dimensional lattices through the Monte Carlo method. We calculate the two-point function at small values of the bare coupling constant and near the continuum limit at finite volume.

(68) **Fantoni R.** and Klauder J. R., Phys. Rev. D **104**, 054514 (2021)
Title: Monte Carlo evaluation of the continuum limit of the two-point function of two Euclidean Higgs real scalar fields subject to affine quantization
Abstract: We study canonical and affine versions of the quantized covariant Euclidean Higgs scalar fieldtheory for two real fields on four dimensional lattices through the Monte Carlo method. We calculate the two-point function near the continuum limit at finite volume.

(69) **Fantoni R.**, Maestre M. A. G., and Santos A., J. Stat. Mech. P103210 (2021)
Title: Finite-size effects and thermodynamic limit in one-dimensional Janus fluids
Abstract: The equilibrium properties of a Janus fluid made of two-face particles confined to a one-dimensional channel are revisited. The exact Gibbs free energy for a finite number of particles N is exactly derived for both quenched and annealed realizations. It is proved that the results for both classes of systems tend in the thermodynamic limit ($N \to \infty$) to a common expression recently derived (Maestre M A G and Santos A 2020 J Stat Mech

063217). The theoretical finite-size results are particularized to the Kern–Frenkel model and confirmed by Monte Carlo simulations for quenched and (both biased and unbiased) annealed systems.

(70) **Fantoni R.**, Mol. Phys. accepted (2021)
Title: Jellium at finite temperature
Abstract: We adopt the fixed node restricted path integral Monte Carlo method within the "Worm algorithm" to simulate Wigner's Jellium model at finite, non zero, temperatures using free-particle nodes of the density matrix. The new element is that we incorporate theWorm algorithm paradigm of Prokof'ev and Svistunov in order to more efficiently handle the fermionic exchanges. We present results for the structure and thermodynamic properties of the ideal Fermi gas and three points for the interacting electron gas. We treat explicitly the case of the partially polarized electron gas.

(71) **Fantoni R.** and Klauder J. R., Int. J. Mod. Phys. A **37**, 2250029 (2022)
Title: Eliminating Nonrenormalizability Helps Prove
Scaled Affine Quantization of φ_4^4 is Nontrivial
Abstract: Following a modest comparison between canonical and affine quantization, which points to positive features in the affine procedures. We prove through Monte Carlo analysis that the covariant euclidean scalar field theory, φ_n^r, where r denotes the power of the interaction term and $n = s+1$ where s is the spatial dimension and 1 adds imaginary time, such that $r = n = 4$ can be acceptably quantized using scaled affine quantization and the resulting theory is nontrivial, unlike what happens using canonical quantization.

(72) **Fantoni R.** and Klauder J. R., Int. J. Mod. Phys. A **37**, 2250094 (2022)
Title: Kinetic Factors in Affine Quantization and Their Role in Field Theory Monte Carlo
Abstract: Affine quantization, which is a parallel procedure with canonical quantization, needs to use its principal quantum operators, most simply $D = (PQ+QP)/2$ and $Q \neq 0$, to represent appropriate kinetic factors, normally P^2, which involve only one canonical quantum operator. The need for this requirement stems from the quantization of selected problems that require affine quantization to achieve valid Monte Carlo results. This task is resolved for introductory examples as well as examples that involve scalar quantum field theories.

(73) **Fantoni R.**, in preparation (2021)
Title: Scaled Affine Quantization of φ_3^{12} is Nontrivial
Abstract: We prove through Monte Carlo analysis that the covariant euclidean scalar field theory, φ_n^r, where r denotes the power of the interaction term and $n = s+1$ where s is the spatial dimension and 1 adds imaginary time, such that $r = 12, n = 3$ can be acceptably quantized using scaled affine quantization and the resulting theory is nontrivial, unlike what happens using canonical quantization.

(74) **Fantoni R.** and Klauder J. R., Eur. Phys. J. C **82**, 843 (2022)
Title: Scaled Affine Quantization of φ_4^4 in the Low Temperature Limit
Abstract: We prove through Monte Carlo analysis that the covariant euclidean scalar field theory, φ_n^r where r denotes the power of the interaction term and $n = s+1$ where s is the spatial dimension and 1 adds imaginary time, such that $r = n = 4$ can be acceptably quantized using scaled affine quantization and the resulting theory is nontrivial and renormalizable even at low temperatures in the highly quantum regime.

Books

(1) **Fantoni R.** "Regole di somma in un gas di elettroni stratificato" ISBN 978-889-101-539-6

(2) **Fantoni R.** "Classical liquids: exact results, integral equations theory, and Monte Carlo simulations" ISBN 978-889-101-543-3

(3) **Fantoni R.** "The Janus Fluid" SpringerBriefs in Physics, (2013), ISBN 978-3-319-00406-8

Schools and Conferences

1994 Napoli CNR meeting. **Poster** on publication (1).

2002 National school of Matter Physics on "Fisica di base delle Nanostrutture e Calcolo ed Informazione Quantistica" (Torino, Villa Gualino, Italy, 9-20 September).

2002 School on "Fisica Statistica, Teoria della Probabilità e Complessità computazionale" (Trieste, ICTP, Italy, 26 August-7 September).

2003 XXII Fai della Paganella meeting: "Fisica Teorica e Struttura della Materia". **Posters** on publication (4) and on publication (5).

2004 XXIII Fai della Paganella meeting: "Fisica Teorica e Struttura della Materia". **Poster** on publication (6).

2004 "IX Convegno Nazionale di Fisica Statistica e dei Sistemi Complessi" (Parma, Italy, 22-24 June). **Contributed Talk** on publication (8).

2004 IV Giovanni Paladin Memorial: "Statistical Mechanics, Chaos and Condensed Matter Theory" (Rome, Italy, 22-24 September). **Poster** on publication (9).

2005 "X Convegno Nazionale di Fisica Statistica e dei Sistemi Complessi" (Parma, Italy, 29-1 July). **Poster** on publications (9) and (10).

2005 "6th Liquid Matter Conference" (Utrecht, the Netherlands, 2-6 July). **Poster** on publications (9) and (10).

2006 "31st Conference of the Middle European Cooperation in Statistical Physics" (Primošten, Croatia, 23-26 April). **Poster** on publication (10).

2007 "Fluid phase behaviour and critical phenomena from liquid state theories and simulations" (CECAM, Lyon, France, 12 July). **Contributed Talk** on publications (14) and (15).

2007 "Statphys23" (Genova, Italy, 9-13 July). **Poster** on publications (14) and (15).

2008 "7th Liquid Matter Conference" (Lund, Sweden, 27 June-1 July). **Poster** on publications (14) and (15).

2009 "Long-range Interactions in Classical and Quantum Physics" (Stellenbosch, South Africa, 16-27 November). **Invited Talk** on publication (17).

2010 "21st Chris Engelbrecht Summer School in Theoretical Physics" (Stellenbosch, South Africa, 18-27 January).

2010 "35th Conference of the Middle European Cooperation in Statistical Physics" (Abbaye des Prómontrés, Pont-à-Mousson, France, 15-19 March). **Poster** on publication (16), (18), and (20).

2010 "Statphys24" (Cairns, Australia, 19-23 July). **Contributed Talk** on publication (17).

2010 **Invited Talk** at the University of Extremadura in Badajoz on publications (16), (18), (20), (21), and (24).

2011 "22st Chris Engelbrecht Summer School in Theoretical Physics" (Stellenbosch, South Africa, 19-30 January).

2011 "Equilibration and Equilibrium 2nd Stellenbosch Workshop on Statistical Physics" (Stellenbosch, South Africa, 7-18 March). **Invited Talk** on publication (24).

2011 "Workshop on Frontiers in Ultracold Fermi Gases" (Trieste, ICTP, Italy, 6-10 June). **Poster** on publications (33) and (39).

2011 "8th Liquid Matter Conference" (Vienna, Austria, 6-10 September). **Poster** on publications (23) and (24).

2011 "National Institute for Theoretical Physics of South Africa (NITheP)" (Stellenbosch, South Africa, 21 Sptember). **Invited Talk** on publication (23).

2011 "International Workshop on Ultracold Molecules" (Stellenbosch, South Africa, 7-11 November).

2012 "XCVIII Congresso Nazionale SIF" (Napoli, Italy, 17-21 September). **Contributed Talk** on publication (30).

2013 "38st Conference of the Middle European Cooperation in Statistical Physics" (Trieste, Italy, 25-27 March). **Poster** on publications (34) and (39).

2013 "Italian National Conference on Condensed Matter Physics (FisMat 2013)" (Milano, Italy, 9-13 September). **Contributed Talk** on publication (41).

2013 "XCIX Congresso Nazionale SIF" (Trieste, Italy, 23-27 September). Abstract on Publication (36) and (40).

2013 **Invited Talk** at the University of Extremadura in Badajoz on publications (41).

2014 "Sigma-Phi-2014" (Rhodes, Greece, 7-11 July). **Chairman** and **Contributed Talk** on publication (43) and (44).

2015 "Italian National Conference on Condensed Matter Physics (FisMat 2015)" (Palermo, Italy, 28 September-2 October). **Contributed Talk** on publication (46).

2017 **Invited Talk** at the University of Extremadura in Badajoz on publication (60).

2017 "Workshop on Understanding Quantum Phenomena with Path Integrals: From Chemical Systems to Quantum fluids and Solids (smr 3131)" (Trieste, ICTP, 3-7 July). Partecipant.

2017 "10th Liquid Matter Conference" (Ljubljana, Slovenia, 17-21 July). **Poster** on publications (55).

2017 "Italian National Conference on Condensed Matter Physics (FisMat 2017)" (Trieste, Italy, 1-5 October). **Talk** on publication (55).

2018 "6th World Congress and Expo on Nanotechnology and Material Science" (Valencia, Spain, 16-18 April). **Invited Talk** on publication (59).

Supervision of PhD thesis

2010 Cosupervision of the Ph.D. thesis of Joris W. O. Salari in the department of polymer chemistry of the University of Technology of Eindhoven in the Netherlands. Supervisor: Prof. Bert Klumperman. Title: "Pickering emulsions, colloidosomes & micro-encapsulation"

2017 Cosupervision of the Ph.D. thesis of Miguel A. G. Maestre in the physics department of the University of Extremadura in Spain. Supervisor: Prof. Andrés Santos. Title: "Structural and thermophysical properties of models of Janus particles with fixed orientation."

Scientific software available to the international scientific comunity

- Development of a Mathematica notebook which evaluates the radial distribution functions for binary mixtures of nonadditive hard spheres, according to the method described in R. Fantoni and A. Santos, "Nonadditive hard-sphere fluid mixtures. A simple analytical theory", Phys. Rev. E **84**, 041201 (2011).
- Development of a Gibbs Ensemble Monte Carlo algorithm to determine the phase properties of a ionic fluid of non-additive hard spheres, according to the method described in R. Fantoni and G. Pastore "Monte Carlo simulation of the nonadditive restricted primitive model of ionic fluids: Phase diagram and clustering", Phys. Rev. E **87**, 052303 (2013).
- Development of a new Quantum Monte Carlo algorithm to determine the phase properties of a quantum fluid of bosons, according to the method described in R. Fantoni and S. Moroni, "Quantum Gibbs ensemble Monte Carlo", J. Chem. Phys. **141**, 114110 (2014).

Other activities

- reviewer for the American Mathematical Society (AMS)
- reviewer for the American Physical Society (APS)
- reviewer for the American Institute of Physics (AIP)

- reviewer for the Institute of Physics (IOP)
- reviewer for the Royal Society of Chemistry (RSC)
- member of SAIP
- member of SIF
- member of EPS
- ranked C3 by the National Research Foundation of South Africa (Division of Research Development) in 2011

Responsibility in projects of supercomputing

1995-2000 Use of the facilities of NCSA at Urbana/Champaign, Illinois, U.S.A.

2010-2012 Use of the facilities of CHPC at Cape Town, South Africa

2011-now Use of the facilities of CINECA at Bologna, Italy