

Workshop on Understanding Quantum Phenomena with Path Integrals: From Chemical Systems to Quantum fluids and Solids | (smr 3131)

Monday, 3 July 2017

08:30 - 23:00 Morning Chairman: Michele CERIOTTI / Afternoon Chairman: Davide GALLI

Location: Adriatico Guest House - Kastler Lecture Hall

08:30 **REGISTRATION & ADMINISTRATIVE FORMALITIES** 1h30'

*Visitors accommodated in the ICTP Guest Houses:
Registration will be done upon check-in at the Guest House reception desk
ONLY Visitors receiving financial support from the ICTP, should go directly to the Operations & Travel Unit office at the Enrico Fermi Building, first floor from 8.30 - 10.00 am, on Monday morning to collect your expenses (after you have registered)*

*Visitors NOT accommodated in the ICTP Guest Houses:
Please register with the Secretariat in office no. 1 at the Adriatico Guest House, lower level 1*

Associateship/Federation scheme Visitors should register at the Leonardo Building, first floor, rooms 112 / 114 / 118

Upon your arrival, please make sure to pick up your Conference Folder in your mailbox at the Adriatico Guest House, lower level 1

10:00 **WELCOME ADDRESSES** 30'

10:30 **Role of the Interaction Core in the Excitation Spectrum of 1D Gases and Liquids** 50'

Speaker: Davide E. GALLI (Universita' degli Studi di Milano, Italy)

Material:  **Abstract**

11:20 **Nuclear Quantum Effects by Accelerated Molecular Dynamics and Quantum Monte Carlo** 50'

Speaker: Sandro SORELLA (SISSA, Trieste, Italy)

Material:  **Abstract**

12:10 **Spatio-Temporal Correlations across the Melting of Wigner Molecules** 20'

Speaker: Amit GHOSAL (IISER, Kolkata, India)

Material:  **Abstract**

12:30 **Lunch break** 2h30' (Adriatico Guest House Cafeteria)

15:00 **Coupled Electron-Ion Monte Carlo Study of Hydrogen under Extreme Conditions** 50'

Speaker: Carlo PIERLEONI (Università degli Studi dell'Aquila, Italy)

Material:  **Abstract**

15:50 **Quantum Solvation: Hydrogen-Bonding and Chemical Reactions in Superfluids** 50'

Speaker: Dominik MARX (Ruhr-Universität Bochum, Germany)

Material:  **Abstract**

16:40 **Coffee break** 30' (Terrace - Adriatico Guest House)

17:10 **Quantum Symmetry from Enhanced Sampling: A First Exploration** 50'

Speaker: Marco NAVA (ETH, Lugano, Switzerland)

Material:  **Abstract**  **Slides**

18:30 **Welcome Get-Together Drink** 2h0' ()















PLEASE NOTE VENUE:
Adriatico Guest House CAFETERIA (inside)

Tuesday, 4 July 2017

- 09:00 - 18:00 Morning Chairmen: Tom MARKLAND & Jeremy RICHARDSON / Afternoon Chairman: Tommaso COMPARIN
- 09:00 **Path Integral Monte Carlo Simulations of Warm Dense Matter 50'**
Speaker: Burkhard MILITZER (University of California, Berkeley, U.S.A.)
Material: [Abstract](#)
- 09:50 **Quantum Dynamics and Spectroscopy of Ab Initio Aqueous Solutions: the Interplay of Nuclear and Electronic Quantum Effects 50'**
Speaker: Ondrej MARSALEK (Stanford University, U.S.A.)
Material: [Abstract](#)
- 10:40 **Coffee break 30'** (Terrace - Adriatico Guest House)
- 11:10 **One-Dimensional Soft Bosons across the Liquid - Cluster Liquid Transition 50'**
Speaker: Gianluca BERTAINA (University of Milan)
Material: [Abstract](#)
- 12:00 **Constructing High-Dimensional Neural Network Potentials (NNPs) to describe the Solvation of Protonated Water Clusters by Superfluid Helium 20'**
Speaker: Christoph SCHRAN (Ruhr-Universitaet Bochum, Germany)
Material: [Abstract](#)
- 12:20 **Lunch break 1h55'** (Adriatico Guest House Cafeteria)
- 14:15 **Path Integral Monte Carlo Calculations of Atomic Bose Gases 50'**
Speaker: Markus HOLZMANN (Grenoble & LPMMC, Paris, France)
Material: [Abstract](#)
- 15:05 **A Diagrammatic Approach to Composite, Rotating Impurities 20'**
Speaker: Giacomo BIGHIN (IST, Klosterneuburg, Austria)
Material: [Abstract](#)
- 15:25 **Coffee break 30'** (Terrace - Adriatico Guest House)
- 15:55 **Proton Coherent Delocalization in the Ground State of Nanoconfined Water 50'**
Speaker: George REITER (University of Houston, U.S.A.)
Material: [Abstract](#)

Wednesday, 5 July 2017

- 09:00 - 21:00 Morning Chairmen: Ondrej MARSALEK & Marco NAVA / Afternoon Chairmen: Nancy MAKRI & Sebastiano PILATI
- 09:00 **Hydrogen Diffusion and Lithium Isotope Fractionation: Cases of Competing and (sometimes) Surprising Quantum Effects 50'**
Speaker: Mark TUCKERMAN (New York University, U.S.A.)
Material: [Abstract](#)
- 09:50 **Path Integral Methods for Nonadiabatic Dynamics: Quantum Transitions from Classical Trajectories 50'**
Speaker: Nandini ANANTH (Cornell University, Ithaca, U.S.A.)
Material: [Abstract](#)
- 10:40 **Coffee break 30'** (Terrace - Adriatico Guest House)
- 11:10 **Rigorous Quantum-Classical Path Integral Formulation of Real-Time Dynamics 50'**
Speaker: Nancy MAKRI (University of Illinois, Urbana, U.S.A.)
Material: [Abstract](#)

- 12:00 **High Order Path Integrals Made Easy** 20'
Speaker: Venkat KAPIL (EPFL, Lausanne, Switzerland)
Material:  [Abstract](#)
- 12:20 **Lunch break** 1h55' (Adriatico Guest House Cafeteria)
- 14:15 **An Electronically Coarse Grained Model describes Water's Properties from Ice to the Supercritical Regime** 50'
Speaker: Glenn J. MARTYNA (IBM - Thomas J. Watson Research Center, Yorktown Heights, U.S.A.)
Material:  [Abstract](#)
- 15:05 **Quantum Transport of Ions through Atomically Thin Materials** 50'
Speaker: Igor POLTAVSKYI (University of Luxembourg)
Material:  [Abstract](#)
- 15:55 **Coffee break** 30' (Terrace - Adriatico Guest House)
- 16:25 **Hanbury Brown-- Twis Effect in Finite-Sized Bose Gases** 20'
Speaker: Daniel SCHUMAYER (University of Otago, Dunedin, New Zeland)
Material:  [Abstract](#)
- 16:45 **Flash Talks Session** 1h15'
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- 16:45 - Superfluidity in a System of Polarized Dipolar Bosons 4'
Speaker: Raul BOMBIN ESCUDERO (Universitat Politecnica de Catalunya)
Material: [Abstract](#) 
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- 16:49 - Analysis and Benchmark of Non-Adiabatic Dynamics with NRPM 4'
Speaker: Danilo CALDERINI (ETH Zurich)
Material: [Abstract](#) 
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- 16:53 - Thermal Field Theory of Bosonic Gases with Finite-Range Effective Interaction 4'
Speaker: Alberto CAPPELLARO (University of Padova)
Material: [Abstract](#) 
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- 16:57 - A Semiclassical Divide-and-Conquer Method for Spectroscopic Calculations of High Dimensional Molecular Systems 4'
Speaker: Giovanni Di LIBERTO (University of Milano)
Material: [Abstract](#) 
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- 17:01 - Quantum and Thermal Effects in the Melting of Simple Solids 4'
Speaker: Marisa DUSSEAULT (Memorial University of St. John's)
Material: [Abstract](#) 
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- 17:05 - Hydrogen Atom Abstraction from Ethanol by Atomic Hydrogen in Aqueous Solution 4'
Speaker: Suraj KANNATH (Lodz Unviersity of Technology)
Material: [Abstract](#) 
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- 17:09 - Inclusion of Quantum Nuclear Effects in Alkanes using PIMD Techniques 4'
Speaker: Nikolay KONDRATYUK (National Research University, Higher School of Economics)
Material: [Abstract](#) 
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- 17:13 - Nuclear Quantum Effects on Surface-Assisted Water Dissociation 4'
Speaker: Yair LITMAN (Fritz Haber Institute, MPI)
Material: [Abstract](#) 
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- 17:17 - Spin Dynamics in One-Dimensional Bosonic Quantum Gases 4'
Speaker: Luca PARISI (University of Trento)
Material: [Abstract](#) 
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- 17:21 - Nuclear Quantum Effects on Acid Dissociation in Microsolvation Environments 4'
Speaker: Ricardo PEREZ de TUDELA (Ruhr-Universitaet Bochum)
Material: [Abstract](#) 
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17:25 - Nuclear Quantum Effects in an HIV/Cancer Inhibitor: The Case of Ellipticine 4'
Speaker: Subrahmanyam SAPPATI (Indian Institute of Science Education & Research)

Material: [Abstract](#) 

17:29 - From Quantum Fluids to Emergent Gravity: Quantum Potential Induced Non-Local BEC & Analogue Hawking Radiation 4'

Speaker: Supratik SARKAR (Indian Institute of Science Education & Research)

Material: [Abstract](#) 


17:33 - Negativity of Wigner Function as Measure of Quantum Correlations 4'

Speaker: Fatima-Zahra SIYOURI (University of Rabat)

Material: [Abstract](#) 


17:37 - Signatures of Inequivalent Representations in Path Integrals 4'

Speaker: Luca SMALDONE (University of Salerno)

Material: [Abstract](#) 

17:41 - Efficient Simulation of Non-Markovian Open Systems using Real Time Path Integrals 4'

Speaker: Aidan STRATHEARN (University of St. Andrews)

Material: [Abstract](#) 


17:45 - Path Integral Methods to Compute Electron Transfer Reaction Rates 4'

Speaker: Manish THAPA (ETH Zurich)

Material: [Abstract](#) 


17:49 - Relaxation Dynamics in Isolated and Open Many-Body Quantum Systems 4'

Speaker: Llinersy URANGA PINA (Universidad de la Habana)

Material: [Abstract](#) 

17:53 - Microcanonical Instanton Rate Theory Applied to Molecular Reactions 4'

Speaker: Pierre WINTER (ETH Zurich)

Material: [Abstract](#) 


17:57 - Nuclear Quantum Effects and Isotope Effects for Vaporation of Dibromomethane 4'

Speaker: Luis VASQUEZ (Lodz University of Technology)

Material: [Abstract](#) 

18:01 - Thermodynamics of the Unitary Bose Gas from First Principles 4'

Speaker: Tommaso COMPARIN (ENS, INO-CNR BEC Center & Univ. di Trento)

Material: [Abstract](#) 

18:05 - Adsorption of Molecular Hydrogen on Nanostructured Surfaces 4'

Speaker: Aliezer MARTINEZ MESA (University of Havana)

Material: [Abstract](#) 

18:15 **Poster Session with Refreshments (outside the Kastler Lecture Hall, lower level) 2h0'**

Thursday, 6 July 2017

09:00 - 23:00 Morning Chairmen: Markus HOLZMANN & Daniel SCHUMAYER / Afternoon Chairman: Guglielmo MAZZOLA

Location: Adriatico Guest House - Kastler Lecture Hall

09:00 **Bound State of a ^3He Atom at ^4He Crystal-Superfluid Interfaces 50'**

Speaker: Massimo BONINSEGNI (University of Alberta, Edmonton, Canada)

Material: [Abstract](#) 

09:50 **Many-body Physics of Superfluid Dipolar Filaments 50'**

Speaker: Fabio CINTI (STIAS, Stellenbosch, South Africa)

Material: [Abstract](#) 

10:40 **Group Photo & Coffee break 30'** (Terrace - Adriatico Guest House)

- 11:10 **Better Variational Density Matrices 50'**
 Speaker: Bryan CLARK (University of Illinois, Urbana, U.S.A.)
 Material: [Abstract](#)
- 12:00 **Quantum Effects in the Bulk Modulus of Solid Molecular Hydrogen 20'**
 Speaker: Bráulio Gabriel BRITO (UFTM, Uberaba, Brazil)
 Material: [Abstract](#)
- 12:20 **Lunch break 1h55'** (Adriatico Guest House Cafeteria)
- 14:15 **Quantum Critical Dynamics in the Relativistic (2+1)-Dimensional Field Theory 50'**
 Speaker: Nikolai PROKOF'EV (University of Massachusetts, Amherst, U.S.A.)
 Material: [Abstract](#)
- 15:05 **Quantum Phase Transitions in 4He Layers Adsorbed on Carbon Allotropes 50'**
 Speaker: Yongkyung KWON (Konkuk University, Seoul, Korea)
 Material: [Abstract](#) [Slides](#)
- 15:55 **Coffee break 30'** (Terrace - Adriatico Guest House)
- 16:25 **Path Integral Estimation of Complex-time Correlation Functions 50'**
 Speaker: Jordi BORONAT (UPC, Barcelona, Spain)
 Material: [Abstract](#)
- 19:00 **Welcome Buffet Reception/Dinner (outside on the terrace, weather permitting) 2h0'** ()

Friday, 7 July 2017

- 09:00 - 14:00 Morning Chairmen: George REITER & David CEPERLEY
- 09:00 **Anharmonic and Quantum Effects in H-bonded Systems with First-principles Accuracy 50'**
 Speaker: Mariana ROSSI (Fritz Haber Institute, Berlin, Germany)
 Material: [Abstract](#)
- 09:50 **Quantum Dynamics, Tunnelling and Electron Transfer beyond Marcus Theory 50'**
 Speaker: Jeremy RICHARDSON (ETH, Zurich, Switzerland)
 Material: [Abstract](#)
- 10:40 **Coffee break 20'** (Terrace - Adriatico Guest House)
- 11:00 **Quantum Monte Carlo Tunneling from Quantum Chemistry to Quantum Annealing 50'**
 Speaker: Guglielmo MAZZOLA (ETH, Zurich, Switzerland)
 Material: [Abstract](#)
- 11:50 **Understanding Quantum Annealing using Projective Monte Carlo Algorithms 20'**
 Speaker: Estelle Maeva INACK (SISSA, Trieste, Italy)
 Material: [Abstract](#)
- 12:10 **Closing Remarks 10'**