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Molecular Electron Dynamics investigated by Intense Fields and Attosecond Pulses



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Home institution

The Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy (MBI) is a non-profit research institution, organized in the legal form of a registered association (Forschungsverbund Berlin e.V.). The MBI is scientifically independent but without legal personality. It is at the same time member of the Leibniz Gemeinschaft and is funded (50% each) by the German federal government (BMBF) and the German states (Länder), in particularly by Berlin. MBI is located at Berlin-Adlershof, City for Science, Technology and Media, one of Germany's major technology parks and a focal point for science, innovative enterprises and media in the region of the German capital. It is positioned in the South-East of Berlin.

The MBI maintains close scientific relations with the three Berlin universities. Its directors are jointly appointed by the institute and one of the universities. Marc Vrakking is full professor at FU-Berlin, Stefan Eisebitt at TU-Berlin and Thomas Elsässer at HU zu Berlin.

The institute was founded by the end of 1991 and consists presently of about 180 members of staff, among them 90 scientists (including guest scientists and PhD students).

The MBI conducts basic research in the field of nonlinear optics and ultrafast dynamics of the interaction of light with matter and pursues applications that emerge from this research. It develops and uses ultrafast and ultra-intense lasers and laser-driven short-pulse light sources in a broad spectral range in combination with methods of nonlinear spectroscopy.

MBI's research program focuses on new sources for ultra-short and ultra-intense light pulses, pulse shaping, pulse characterization, measuring techniques for ultra-fast processes in a broad spectral range from the mid-infrared to the x-ray region, ultrafast and nonlinear phenomena with special emphasis on atoms, molecules, clusters and plasmas and surfaces and solid state.

With its research the MBI fulfills a nationwide mission and is an integral part of the international science community. The MBI is involved in a large number and variety of cooperative research projects with universities, other research institutions and industrial partners.

The research structure of the Max Born Institute comprises 10 research projects and two infrastructure projects, organized in 4 focus areas. Complementary to this, the organizational structure with 3 research divisions (each with 3 departments) defines the key fields of scientific competence of MBI-scientists and the corresponding scientific equipment.

The combination of modern laser development and measuring technique with its interdisciplinary application in basic research and for emerging key technologies constitutes the unique profile of the MBI and its attraction to external cooperation partners.



Group leader

Name: Olga Smirnova Nationality: Russian Date of birth: 12 July 1973

Short CV:

1996: graduated in Physics, Moscow State University, Russia 2000: PhD in Physics, Moscow State University, Russia

Field : Strong Field Interaction with Atoms and Molecules

Research interests: Strong-field and attosecond physics, High Harmonic Spectroscopy, Ultrafast spectroscopy of chiral molecules, Nonlinear dynamics.

Awards:

- 2010 Karl-Scheel-Preis of Physikalischen Gesellschaft zu Berlin
- 2009 SAW award of Leibniz society: funds to establish junior group and maintain it for 3 years
- 2003 Lise-Meitner Fellowship of Austrian Science Foundation (FWF)

Current position:

Professor of Physics, Technical University Berlin, Germany Group Leader, Max Born Institute, Berlin, Germany

I was fascinated with physics since I first got hold of a children's book which described how atoms are made of nuclei and electrons. I think that I was about five years old at that time. And since I was 13, I knew that I wanted to be a physicist, and that I wanted to study at the Moscow State University.

When I was a child in what was then the Soviet Union, the status of science and education in the country was high, but by the time I started at the University, the Soviet Union was collapsing and the science and education were disintegrating, as they were no longer among the country's priorities. There was simply no money left.

I graduated in 1996 and started my PhD, looking initially at the signatures of classically chaotic dynamics in nonlinear response of quantum systems to light.

The project looked extremely interesting and exciting, I could eventually see the signatures of chaotic dynamics in the rather complicated analytical expressions for non-linear susceptibilities of chaotic systems, derived after a couple of years of hard work, but the final and ultimate proof required extensive numerical analysis which has not been available at that time. Fortunately, as an aside, I started to look at extreme nonlinear response to really intense laser fields, where the electric field strength is comparable to the electrostatic field that binds electrons in atoms. Such fields completely restructure the atom, dictating the behavior of the electrons. It was this work that has become the central part of my PhD thesis, which I have defended in 2000. This experience has taught me an important lesson: research projects do not always work out the way you originally planned, but even then it will inevitably lead you to new questions and new ideas. Just keep your mind open! Shortly after I obtained my PhD, I started my term as an Assistant Professor teaching and supervising students at the Moscow State University.

My work on extreme nonlinear optics and ultrafast electronic response to intense laser fields has naturally led me to attosecond physics, and in 2003 I left Moscow State University for Vienna, to join one of the world leading attosecond groups as Lise Meitner Fellow. The group was led by Prof. Ferenc Krausz at the Vienna Technical University, and I have joined the theory team of Prof. Armin Scrinzi, who taught me how to appreciate and use the numerical methods. Complementing my expertise in analytical approaches by the new skills in numerical methods was extremely useful and helped me to develop many projects in the future. I have spent two amazing years in Vienna, both scientifically and culturally. For the first time I felt what does it mean to be immersed in the atmosphere created by the people advancing the frontiers of science, the excitement of interacting with these brilliant people and the amazing experiments.

In 2005 I moved to the second world center for attosecond science, in Ottawa, Canada, led by Prof. Paul Corkum at the Steacie Institute for Molecular Sciences of the National Research Council of Canada. There I met many brilliant scientists and had a lot of fun working with them on developing the foundations of high harmonic spectroscopy. High harmonic spectroscopy allows one to make 'movies' of how charges flow between different atoms in a molecule. The 'movies' are made by illuminating the molecule with intense laser light and recording the new light, at much shorter wavelengths, emitted by the molecule. This light encodes the motion of electrons in the molecule with extraordinary temporal resolution: several tens of 'frames' in this movie are fit within a single femtosecond - one billionth of a billionth of a second. What's more, the sub-femtosecond temporal resolution can be combined with spatial resolution of about one angstrom, and this is why we talk about making subfemtosecond 'movies'. In our joint work we have shown how to develop these movies, finding ways to decode the 'images' stored in all properties of the emitted light - its intensity, phase, and polarization. I have made many friends in Canada and I continue to collaborate with them to this day.

In 2006 I have become a permanent staff member at NRC, and in 2008 I have obtained SAW grant to start my own research group at the Max Born Institute in Berlin, Germany. In 2016 I have become a full Professor at the Berlin Technical University, which is a joint appointment with the MBI.

Understanding dynamical processes often relies on our ability to resolve them in time. Attosecond science is developed to open a window into the world of correlated multi-electron dynamics in atoms, molecules, clusters and solids. Our work is a part of this direction. Our research goals include time- and space-resolved imaging and control of electron dynamics such as charge migration, electron rearrangement, autoionization, coupling of electronic and vibrational dynamics in molecules. We develop new tools and ideas that help us image and understand coherent attosecond electron dynamics in molecules.



Institute Director

Name: Marc Vrakking Nationality: Dutch Date of birth: 1 September 1963

Short CV:

1987: graduated in Physics, Technical University of Eindhoven, the Netherland s

1992: PhD in chemistry, University of California Berkeley, USA

Current position:

Professor of Physics, Freie Universität Berlin, Germany Director of the Max Born Institute, Berlin, Germany Professor of Physics, university of Nijmegen, Netherlands Group leader at AMOLF, XUV Physics (until July 2011)

My appetite to become a scientist was wetted at a very early age. As a boy I was fascinated by the stories of my father (a research scientist at the Philips Physics Laboratories in Eindhoven, NL). Life in laboratories seemed challenging and exciting. So, although I considered studying journalism and history, it was no surprise that in the end I chose to study physics. After the first few tedious years my enthusiasm was triggered when I got to work in a real lab. My first summer research project (on the properties of molecular beams made by expanding gas at high pressure through a little hole) led to an offer by my supervisor to spend half a year in a research laboratory in Japan.

At my host laboratory in Japan there were no PhD students, let alone undergraduate students. Since the people there seemed to have forgotten how little undergraduate students know, expectations seemed very, very high. But I went into the lab that I was given, invented my own research project, built some components using fancy machine shop equipment that I've never been allowed to use since (!) and... got really nice results Still, despite the hours that I spent in the lab – which exceeded even those of the Japanese colleagues - the real attraction was also Japan itself. Life far away from home in an exotic country made my stay amazing and utterly fascinating. In the end, Japan was one of the most formative experiences in my life.

Spending time in Japan led to the US. After finishing up my Master's degree in Eindhoven I made my way to Berkeley to pursue my PhD in chemistry in the group of the 1986 Chemistry Nobel laureate Professor Yuan Lee. Berkeley was renowned for its very difficult experiments. Lee certainly had one in mind for me: studying the reaction of H+H2 \rightarrow H2+H using an all-laser experiment. I spent weeks behind my drawing board designing the experiment, then guiding the fabrication of the instruments in the machine shop and building up and testing everything (including one of the first photoelectron/photo-ion imaging detectors.) After two and a half years, with every individual component finally working, the quality of the data proved insufficient to draw any important new conclusions. That was a massive disappointment, but it taught the importance of structuring your research program: providing enough intermediate results and milestones-alongthe-way to feed your resume and not to dash for the muchanticipated finish line. Fortunately during my last year in Berkeley I did some experiments on the side which proved a big hit.

After 5 PhD and 2 post doc years I left Berkeley to spend a year in Ottawa "on my way home", to work with former Berkeleycolleague and good friend Albert Stolow, whose lab was part of the department of Paul Corkum. This brought me into contact with femtosecond laser techniques and many of the concepts that would become so important in my later work: highharmonic generation, the response of molecules to intense laser fields, and - even! - the first thoughts about how one might be able to make attosecond laser pulses. I came back to the Netherlands on a fellowship and shortly thereafter was contracted by AMOLF start my own group. In 1997 I wanted to start a research group using high harmonics to probe time-resolved molecular dynamics. In 2000 we were ready to try pump-probe experiments, with very frustrating results. We managed a few nice publications, but we failed every time when we tried to do a pump-probe experiment with harmonics.

Then the first attosecond paper came out (in Science), following an idea from my AMOLF-colleague Harm-Geert Muller. A major result with just one little side note: why hadn't Harm-Geert done the experiment at AMOLF, where we had all the equipment available and ready-to-go!?

To underscore this, we started attosecond experiments at AMOLF, soon becoming the 3rd team to demonstrate them. Though the ideas on what attosecond pulses could be used for were still sketchy, I started/decided to focus on attosecond pulses.

This choice proved right. Attosecond science has developed explosively since then. Ironically, the efforts to develop attosecond experiments (characterizing the pulses and developing setups where they could be used to study time-resolved electron dynamics) solved a lot of the problems that defeated our harmonics-based pump-probe experiments early on. Last year we went back to what in 2000 was supposed to be our first experiment, and it worked like a charm.

A few years ago I decided to accept an offer from the Max Born-Institute in Berlin to become one of its three directors. A tremendous challenge and opportunity. Working in one of Europe's premier centers for ultrafast laser science, where you can live out all your research dreams, was just too good to pass up. At the moment we are busy planning a series of new, state-of-the art laboratories where in the coming years our attosecond research program is going to get underway, with experiments where we'll investigate electronic and atomic dynamics on the fastest possible timescales. Truly something to look forward to!

Offered training

Research Training Modules (RTMs)

- A. Inversion procedure for angular resolved photoelectron measurements (see next pages for details)
- B. Introduction to strong field ionization of atoms and molecules (see next pages for details)

Scientific Courses of the MBI

Ultrafast Laserphysics	Prof. Dr. Mrac Vrakking
Quantum Dynamics in Strong Laser Fields	Prof. Dr. Mikhail Ivanov
Non-Linear Optics	Prof. Dr. Mikhail Ivanov
Theoretische Physik II Elektrodynamik*	Prof Dr. Kurt Busch, Dr. Christian Matyssek
Quantensysteme I, Integrierte LV (VL mit UE)*	Prof Dr. Ulrich Eich- mann, Prof. Dr. Otto Dopfer
Laserphysik*	Dr. Michael Wörner
Modern Experiments in Attosecond Physics	Dr. Oleg Kornilov

Transferable skills Modules (TSMs)

Language course	
Basics of scientific presentation	

* Courses take place in German language

A. Inversion procedure for angular-resolved photoelectron measurements

Objective

In angular resolved momentum measurements of photoelectrons or ions often the velocity map imaging (VMI) technique is used. In cases of cylindrical symmetry, it is sufficient to experimentally project the three-dimensional momentum distribution (r,θ,ϕ) on a spatially resolved, two-dimensional (x,y) detector. The retrieval of the underlying distribution from the measured image requires an appropriate Abel inversion technique. A number of different methods were developed since the invention of VMI, with different strengths and weaknesses. The goal of this RTM is to get to know some of the different procedures and benefit from the practical implementation in a software code at MBI, which we are willing to share with the ESR.



Required Background and Scope

Previous experience with a programming language, ideally Python, is essential. The ESRs will be provided with a desktop computer and a software module, written on Python v 2.x.

The scope of the training encompasses:

- Read in of raw images in a number of different formats
- Pre-processing of images
- Spline-interpolation and projection into different coordinate systems
- Analysis in a basis set, in particular Legendre functions
- Different inversion methods, including Fourier-Hankel, Basex, pBasex, Maximum Entropy Reconstruction, iterative and Monte-Carlo-Reconstruction.

Duration

For the training a period of <u>two to four weeks</u> is planned. Existing or synthesized data will be used for the training. It might also be useful for the RTM to participate in a measurement campaign on photoelectron angular distributions or a related subject at MBI.

The period for the participation to the RTMs should be agreed upon with the tutors.

RTM at a glance

Title	Host institution	Objective	Duration/ Period	Tutors
Inversion procedure for photoelectron angular distributions	МВІ	Utilize different inversion procedures <u>experimental activity</u>	2-4 weeks / to be discussed	Felix Brausse <u>felix.brausse@mbi-berlin.de</u> Arnaud Rouzee <u>arnaud.rouzee@mbi-berlin.de</u> Jochen Mikosch <u>jochen.mikosch@mbi-berlin.de</u>

B. Introduction to strong field ionization of atoms and molecules

Objective

The theory group at the MBI offers training in the theory of intense laser atom and laser molecule interactions. Training can include both analytical and numerical methods for describing strong field ionization and high harmonic generation of atoms and molecules. The student will learn



fundamentals of the key theoretical tools used to describe ionization of atoms and molecules in strong low-frequency laser fields

Equipment and theoretical concepts

The ESR will get hands on training in the single-active electron numerical codes that we use to simulate strong field ionization and high harmonic generation.

We have developed a set of hands-on exercises that allow the student to not only learn the theoretical foundations but also to visualize the studied physics using numerical experiments.

- Basic method for the time-dependent treatment of laser-matter interaction: the time-dependent Schrodinger equation,
- Wavepacket dynamics: spreading and center of mass motion
- Gauges for describing light-matter interaction,
- Strong field ionization in the tunneling and multi-photon regimes
- The Volkov states and the Volkov propagator
- The strong field S-matrix theory, the Strong Field Approximation, and the Analytical R-matrix theory.
- Ionization of atoms and molecules: the role of the initial orbital
- Ionization in circularly polarized laser fields
- Time-resolving strong-field ionization and the attoclock
- Numerical simulations of strong-field ionization: the spectral and the grid methods, various propagators, their strengths and weaknesses,
- Recollision physics and its consequences: high harmonic generation and electron-parent ion diffraction
- Quantum orbits in high harmonic generation
- Multi-channel and multi-electron effects in strong-field ionization
- Multi-channel and multi-electron effects in high harmonic generation
- High harmonic generation spectroscopy of attosecond electron-hole dynamics

Duration

The period for the participation to the RTMs should be agreed upon with the tutors. Depending on the length of the secondment, the hands on training may include running simulations pertinent for solving the problems that we are currently working on.

RTM at a glance

Title	Host institution	Objective	Duration/ Period	Tutors
Introduction to strong field ionization of atoms and molecules	МВІ	Theoretical training in the theory of intense laser atom and laser molecule interactions.	To be discussed	Felipe Morales <u>morales@mbi-berlin.de</u> Mikhail Ivanov <u>mivanov@mbi-berlin.de</u> Olga Smirnova <u>smirnova@mbi-berlin.de</u>



About the life in Berlin

Germany's largest city (population: 3.4 million citizens) provides a wealth of attractive and diverse cultural opportunities. In addition to the free and experimental arts scene, there are 3 large opera houses, 170 museums, 150 theaters and 8 symphony orchestras. Berlin is also a very green city: a quarter of the area is covered by parks and woodlands and almost 200 kilometers of navigable waterways wind their way through the city. The city of Berlin has a special website dedicated to tourism and cultural events in the city to enjoy the city, its culture and its leisure:

http://www.berlin.de/en/

It also provides useful information about the transformation system, how to get tickets, and suggestions for different trips and tours around the city.

Welcome activities at the home institution

If you are visiting the institute you should contact us as soon as possible so we can arrange everything necessary for your visit.

We will then guide you through all steps in order to make your visit as smooth as possible.