INTERNATIONAL WORKSHOP
Correlation and Polarization Phenomena in Ionization of Dilute Species by XUV and X-ray Radiation

MOSCOW 2012

MAY 24-25

SKOBELTSYN INSTITUTE OF NUCLEAR PHYSICS
LOMONOSOV MOSCOW STATE UNIVERSITY

DEUTSCHES ELEKTRONEN-SYNCHROTRON
A RESEARCH CENTRE OF THE HELMHOLTZ ASSOCIATION

GEFÖRDERT VOM
Bundesministerium für Bildung und Forschung

EUROPEAN X-RAY FREE-ELECTRON LASER FACILITY GmbH

CONFERENCE PROGRAM & ABSTRACTS

RUSSIA

INTERNATIONAL WORKSHOP

Correlation and Polarization Phenomena in Ionization of Dilute Species by XUV and X-ray Radiation

Moscow, Russia, 24-25 May 2012

Program and Abstracts

This workshop is the second in a series of meetings of participants of the two projects *"Correlation and Polarization Phenomena in Ionization of Dilute Species by XUV and X-ray Radiation"*(Principal Coinvestigators: A.N. Grum-Grzhimailo and N.M. Kabachnik (Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University), M. Meyer (European XFEL, Hamburg), J. Viefhaus (DESY, Hamburg)) and *"High accuracy measurements of partial photoionization cross sections of rare gases – a crucial database for FEL photon diagnostics"* (Principal Coinvestigators: S.V. Bobashev (Ioffe Institute, Saint Petersburg), M. Richter (PTB, Berlin), A. Sorokin (DESY, Hamburg), K. Tiedtke (DESY, Hamburg). Both projects are funded by the German BMBF within the framework of the German-Russian Cooperation *"Development and Use of Accelerator-Based Photon Sources"*. The first meeting took place in Hamburg on the 21/22 of February, 2011.

This Moscow meeting includes oral presentations and posters on the topics of the projects, describing current state and future plans of the investigations. One of the main aids of the workshop is to discuss and to coordinate further experimental and theoretical activities in order to achieve the best value on the cooperation.

PROGRAM OF RUSSIAN-GERMAN WORKSHOP
"Correlation and Polarization Phenomena in Ionization of Dilute Species by XUV and X-ray Radiation"
Moscow, Russia, 24-25 May 2012

The Workshop will take place in Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University (see the map). All oral presentations on May 24 are in the room 2-15, coffeebreaks are in the room 1-18.

Thursday, May 24, 2012

9.00	**Registration (Room 1-05)**	
9.30	**Opening (Room 2-15)**	
Session 1. General (*Chair: Alexei Grum-Grzhimailo*)		
9.40	*Victor Savrin*	Welcome
10.00	*Uwe Becker*	Coherence and loss of coherence in the photoionization of inversion symmetric systems
10.40	*Markus Ilchen*	Coherence effects in the valence photoionization of small molecules
11.10	*Stephan Fritzsche*	Calculation of atomic ionization and recombination properties in synchrotron and FEL radiation
11.50 – 12.20 Coffee Break (Room 1-18)		
Session 2. Experiment (*Chair: Michael Meyer*)		
12.20	*Andrey Sorokin* *Kai Tiedtke* *Henning Kühn*	Gas-monitor detector for the X-ray regime: first use for characterization and radiometric comparison at SACLA and LCLS FELs
12.50	*Jens Viefhaus*	An update on atomic and molecular physics experiments at the variable polarization XUV beamline P04 at PETRA III
13.20	*Sascha Deinert*	First measurements using the Time of Flight spectrometer for highly efficient electron-ion-coincidence experiments in the XUV-regime
13.40 – 15.10 Launch		
Session 3. Pump-probe Processes: Experiment and Theory (*Chair: Jens Viefhaus*)		
15.10	*Michael Meyer*	Angle-resolved electron spectroscopy of Laser Assisted Auger Decay in atomic Neon
15.40	*Tommaso Mazza*	Controlling core hole relaxation dynamics via intense optical fields
16.10	*Nikolay Kabachnik*	Linear dichroism in short-pulse two-color XUV+IR multiphoton ionization of atoms
16.40 – 17.10 Coffee Break (Room 1-18)		
Session 4. Theory: Nonlinear and Nondipole Effects in the XUV (*Chair: Nikolay Kabachnik*)		
17.10	*Elena Gryzlova*	Manifestation of discrete and autoionizing states in sequential atomic ionization by few XUV photons
17.40	*Anastasia Bityutskaya*	Non-resonant transitions in sequential three-photon double atomic photoionization of noble gases in the XUV
18.00	*Alexei Grum-Grzhimailo*	Beyond the dipole approximation in two-photon ionization at FELs
18.30	*Alexander Galstyan*	Non-dipole effects in (γ, 2e) processes caused by photon momentum
Friday, May 25, 2012 (Room 1-18)		
9.30	Poster Session	
10.30 – 10.50 Coffee Break		
10.50	Discussions within Working Groups and Round Table Discussion	
	Workshop photo	
<18.00	Launch, Sightseeing	
>18.00	Banquet (see the map)	

List of participants

Andrianov	**Victor**	SINP MSU	andrva@srd.sinp.msu.ru
Bakhtiarzadeh	**Sadegh**	European XFEL, Hamburg	sadegh.bakhtiarzadeh@xfel.eu
Bityutskaya	**Anastasiya**	Faculty of Physics, MSU	asybit@yandex.ru
Becker	**Uwe**	FHI, Berlin	becker_u@fhi-berlin.mpg.de
Blokhintsev	**Leonid**	SINP MSU	blokh@srd.sinp.msu.ru
Bobashev	**Sergey**	Ioffe PTI, Saint-Petersburg	s.bobashev@mail.ioffe.ru
Braune	**Markus**	DESY, Hamburg	Markus.Braune@desy.de
Bulychev	**Andrey**	Faculty of Physics, MSU	a.a.letterbox@gmail.com
Deinert	**Sascha**	DESY, Hamburg	sascha.deinert@desy.de
Fritzsche	**Stephan**	GSI, Darmstadt	s.fritzsche@gsi.de
Galstyan	**Alexander**	Faculty of Physics, MSU	galstyan@physics.msu.ru
Glaser	**Leif**	DESY, Hamburg	leif.glaser@desy.de
Grum-Grzhimailo	**Alexei**	SINP MSU	algrgr1492@yahoo.com
Gryzlova	**Elena**	SINP MSU	gryzlova@gmail.com
Ilchen	**Markus**	DESY, Hamburg	markus.ilchen@desy.de
Kabachnik	**Nikolay**	SINP MSU	nkabach@googlemail.ru
Khaerdinov	**Mikhail**	SINP MSU	khaerdinovmn@gmail.com
Kouzakov	**Konstantin**	Faculty of Physics, MSU	kouzakov@srd.sinp.msu.ru
Kühn	**Henning**	DESY, Hamburg	henning.kuehn@desy.de
Markova	**Anastasiya**	Ioffe PTI, Saint-Petersburg	angelinme@mail.ru
Mazza	**Tommaso**	European XFEL, Hamburg	tommaso.mazza@xfel.eu
Meyer	**Michael**	European XFEL, Hamburg	michael.meyer@xfel.eu
Popov	**Yuri**	SINP MSU	popov@srd.sinp.msu.ru
Ryazantsev	**Sergey**	Faculty of Physics, MSU	sergryaz@mail.ru
Seltmann	**Jörn**	DESY, Hamburg	joern.seltmann@desy.de
Strakhova	**Svetlana**	SINP MSU	str@sinp.msu.ru
Sorokin	**Andrey**	DESY, Hamburg	andrey.sorokin@desy.de
Tiedtke	**Kai**	DESY, Hamburg	kai.tiedtke@desy.de
Viefhaus	**Jens**	DESY, Hamburg	jens.viefhaus@desy.de

Coherence and loss of coherence in the photoionization of inversion symmetric systems

Uwe Becker

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The electronic states of inversion symmetric systems such as homonuclear diatomic molecules are eigenstates of the Parity operator, the so-called delocalized gerade and ungerade eigenstates. These states are coherent superpositions of both atomic sites of the molecule giving rise to double slit like oscillations in the photoabsorption cross section of these molecules. These are the well-known Cohen-Fano oscillations [1,2]. A less well-known fact is the characteristic behavior of these oscillations depending whether the electrons are emitted from a randomly distributed or an oriented target. This should give rise to a phase shift of $\pi/2$ between both situations regarding their corresponding Cohen-Fano oscillations. We show this phase shift effect unambiguously for the first time for the photoionization of molecular hydrogen.

More astonishingly is however the phenomenon, that even for the randomly oriented target the oscillatory behavior converts into the one of an oriented target for high photoelectron kinetic energies. This transition between the two behaviors is brought about by the recoil momentum of the photoelectron, which reveals the molecular axis orientation at the moment of its emission. This unexpected effect has been observed for the first time for the case of molecular hydrogen.

Coherent oscillations appear in both the cross section and the angular distribution asymmetry parameter. There was the assumption that these oscillations are closely related, in fact the β-oscillation should be the inverse of the σ-oscillation. We could prove this assumed relationship for the first time unambiguously for the valence photoionization of N_2.

Decoherence occurs if the gerade and ungerade Parity eigenstates are coherently superimposed. This can be either in the decay or excitation process. We have chosen the excitation of the core electron of O_2 to energetically degenerate gerade and ungerade states, which are hence coherently superimposed. This coherent superposition shows up by the Fano profile of the corresponding partial cross section. The coherent superposition of the gerade and ungerade Parity states causes decoherence of the position states and hence localization of the electron emitter site. By choosing two very different decay time scales for the so-called first and second step Auger emission we were able to demonstrate the electron tunneling effect by Doppler shifted electron-fragment ion coincidence experiments as introduced by Kugeler et al. as a tool for studying the behavior of dissociating molecular systems [3]. This complex relationship will be explained in more detail in the talk.

[1] H. D. Cohen and U. Fano Phys. Rev. **150**, 30 (1966)
[2] O. A. Fojon et al. Journal of Physics B **37**, 3035 (2004)
[3] O. Kugeler et al. Phys. Rev. Lett. **93**, 33002 (2004)

Coherence effects in the valence photoionization of small molecules

Markus Ilchen[1], Markus Braune[1,2], Sascha Deinert[1], Leif Glaser[1], André Meissner[2], Frank Scholz[1], Peter Walter[1], Jens Viefhaus[1] and Uwe Becker[2]

[1]*Deutsches Elektronen Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany*
[2]*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany*

Oscillations in the partial photoionization cross sections of homonuclear diatomic molecules have been described by Cohen and Fano more than 40 years ago [1] as an interference phenomenon analogous to a double slit experiment. These cross section oscillations have been verified by several experiments in the meantime. In addition to the cross section however, also the angular distribution asymmetry parameter β, the non-dipole angular distribution parameters and most likely all spin parameters are showing oscillations. The physical reason of these oscillations has not necessarily to be only the partial cross section and such effects could also be caused by phase shifts of the outgoing photoelectron partial waves.
Results for the valence photoionization of molecules such as N_2, O_2 and CH_4 will be presented.

[1] H.D. Cohen and U. Fano, Phys. Rev. **150**, 33 (1966)

Calculation of atomic ionization and recombination properties in synchrotron and FEL radiation

S. Fritzsche

GSI Helmholtzzentrum für Schwerionenforschung, D-64291 Darmstadt, Germany
Department of Physics, University of Oulu, Box 3000, FI-90014 Oulu, Finland

The RATIP program has been developed during the past decade to calculate the electronic structure and properties of atoms and ions [1]. Today, these tools provide a powerful platform for studying atomic processes of open-shell atoms and ions in synchrotron and FEL radiation, including photo excitation, ionization and Auger processes. Although the main focus in developing these tools has been paid on processes with just a single electron in the continuum, recent emphasis was placed also on second-order processes as well as those properties for which different types of (many-electron) amplitudes need to be combined in order to explain complex spectra. In this contribution, I present and discuss the present capabilities of the RATIP tools of which a major part now became public [2]. Further examples refer to the direct and sequential double ionization of various atoms in the gas phase [3,4].

[1] S. Fritzsche, J. Elec. Spec. Rel. Phenom., **114-116**, 1155 (2001)
[2] S. Fritzsche, Comput. Phys. Commun. **183**, 1525 (2012)
[3] P. Linusson et al., Phys. Rev. A **83**, 023424 (2011)
[4] S. Fritzsche, A.N. Grum-Grzhimailo, E.V. Gryzlova and N.M. Kabachnik, J. Phys. B **44**, 175602 (2011)

Gas-monitor detector for the X-ray regime: first use for characterization and radiometric comparison at SACLA and LCLS FELs

A.A. Sorokin[1,2], S.V. Bobashev[2], T. Ishikawa[3] , M. Kato[3,4], H. Kuehn[1], S. Moeller[5], M. Richter[6], A. Robert[5], N. Saito[3,4], K. Tiedtke[1], K. Tono[3], M.Yabashi[3]

[1]*Deutsches Elektronen-Synchrotron, DESY, Notkestrasse 85, D-22603 Hamburg, Germany*
[2]*Ioffe Physico-Technical Institute, Polytekhnicheskaya 26, 194021 St. Petersburg, Russia*
[3]*SPring-8/RIKEN, 1-1-1 Kouto, Sayo-cho, Sayo-gun, Hyogo 679-5148, Japan*
[4]*National Institute of Advanced Industrial Science and Technology (AIST), NMIJ, Tsukuba 305-8568, Japan*
[5]*SLAC National Accelerator Laboratory, Stanford, CA 94309, USA*
[6]*Physikalisch-Technische Bundesanstalt, PTB, Abbestrasse 2-12, D-10587 Berlin, Germany*

During the last years an impressive progress has been achieved in the development of next generation powerful short wavelength sources like self-amplified spontaneous-emission free-electron lasers (FELs), opening the door for new investigations of photon matter interaction on nanometer and femtosecond scales. The first such source was the Free-electron LASer in Hamburg (FLASH) which operates in the extreme ultra-violet range (EUV) from 48 down to 4.3 nm. Recently, two X-Ray facilities were put into operation: the X-ray FEL Linac Coherent Light Source (LCLS) in USA operated at wavelengths between 2.4 nm and 0.15 nm and the SPring-8 Angstrom Compact free-electron Laser (SACLA) in Japan, which reached laser amplification up to photon energy of 17 keV. Moreover, new X-ray FEL facilities in Germany (European XFEL) and Switzerland (PSI) are currently under construction. However, in spite of the evident progress in the development of laser facilities, the characterization of FEL beam parameters like the photon flux, which is one of the most important beam qualities, is a great challenge because the highly intense and strongly pulsed FEL beam with a peak power of up to a few GW can easily saturate or even destroy solid state detectors commonly used at synchrotron facilities. Moreover, each FEL pulse is different with respect to the number of photons, requiring on-line monitoring of the pulse intensity for the FEL operators and experimenters. In order to overcome these challenges we developed gas-monitor detectors (GMDs) of different types within the framework of German-Russian collaboration. The operation of the GMDs is based on the photoionization of rare gases or molecules at low pressure. Hence, the accurate determination of the FEL beam intensity relies on the GMDs calibration performed in the vacuum-ultraviolet spectral range using synchrotron radiation at low intensity in conjunction with a cryogenic radiometer as the primary detector standard as well as on the utilization of total and partial photoionization (PI) cross section data of the target gas to extrapolate the calibration data to EUV and X-ray regime. Therefore, the knowledge of the PI cross sections with low uncertainty is mandatory for accurate operation of the GMDs at existing and upcoming EUV and X-ray FEL facilities.

Here, we describe the operation principles of recently developed GMD for the European XFEL and its first use in the X-ray regime for characterization of the LCLS and SACLA FELs as well as a direct radiometric comparison with alternative detectors used at the latter facilities. Furthermore, we present an actual status of the Russian-German project on precise measurements of the partial PI cross sections of rare gases and small molecules in the X-ray regime.

An update on atomic and molecular physics experiments at the variable polarization XUV beamline P04 at PETRA III

Jens Viefhaus, Sascha Deinert, Leif Glaser, Markus Ilchen, Frank Scholz, Jörn Seltmann, Ivan Shevchuk, Beata Terka, and Peter Walter

Deutsches Elektronen Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

After the introduction of the PETRA III facility including its substantial extension project an overview about recent and planned experimental activities in the field of atomic and molecular physics at the XUV beamline P04 will be given. Special emphasis is put on those experiments which are part of the German Russian BMBF project including coincidence experiments, non-dipole and two-colour measurements. Future activities will be discussed in the frame of exploratory experiments already performed at BESSY II (HZB, Berlin) and DORIS III (DESY, Hamburg).

First measurements using the Time of Flight spectrometer for highly efficient electron-ion-coincidence experiments in the XUV-regime

Sascha Deinert, Leif Glaser, Markus Ilchen, Frank Scholz, Jörn Seltmann, Peter Walter and Jens Viefhaus

Deutsches Elektronen Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

A new time-of-flight spectrometer was developed and optimized with emphasis on electron-ion-coincidence experiments at the P04 Polarization XUV Beamline at PETRA III (DESY/Hamburg). It comprises of a very short time-of-flight spectrometer for ion detection, based on the concepts of Wiley and McLaren [1] using electric fields, and a so called magnetic bottle electron spectrometer, which was described by Kruit and Read [2]. The combination of these two devices for coincidence measurements of ions and electrons is already in use e.g. by Eland and Feifel [3]. However, our electro- and magneto-static simulations (using a combination of Simion [4] and Radia [5] software packages, respectively) have shown that there is space for improvements

We present the principle of operation with the help of simulation, the current status of the development and first results including the comparison of simulation data and measurements on atoms and small molecules obtained by using different light sources at DESY/Hamburg.

[1] W.C. Wiley and I.H. McLaren, Rev. Sci. Instrum. **26**, 1150 (1955)
[2] P. Kruit and F.H. Read, J. Phys. E **16**, 313 (1983)
[3] J. H. D. Eland and R. Feifel, Chemical Physics **327**, 85 (2006)
[4] D. Dahl, Int. J. Mass Spectrom. **200**, 3 (2000)
[5] O. Chubar, P. Elleaume, J. Chavanne, J. Synchrotron Rad. **5**, 481 (1998)

Angle-resolved electron spectroscopy of Laser Assisted Auger Decay in atomic Neon

M. Meyer,[1] P. Radcliffe,[1] J.T. Costello,[2] S. Düsterer,[3] A.K. Kazansky,[4] and N.M. Kabachnik[1,5]

[1] *European XFEL GmbH, Albert-Einstein-Ring 19, D-22761 Hamburg, Germany*
[2] *School of Physical Sciences and NCPST, Dublin City University, Dublin 9, Ireland*
[3] *HASYLAB at DESY, Notkestrasse 85, D-22607 Hamburg, Germany*
[4] *Donostia International Physics Centre (DIPC), E-20018 San-Sebastian/Donostia, Spain*
[5] *Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Leninskie Gory, Moscow, 119234, Russia*

Photoionization and subsequent Auger decay are the dominant processes after the interaction of atoms with photons of short wavelength. New possibilities to obtain dynamical information about this extremely fast process were opened up in the last years due to the development of Free Electron Lasers, such as FLASH in Hamburg and LCLS in Stanford, with their unprecedented characteristics, especially the ultra-short temporal width of the pulses, which can be as short of a few femtoseconds, and the extremely high number of photons per pulse (about 10^{12}-10^{13} photons/pulse). In a series of experiments at LCLS, we have taken advantage of the very short (2-5fs) pulse durations, which are delivered by this new X-ray Free Electron Laser. This temporal width coincides with the lifetime of core hole states governing the dynamics of the Auger decay, and with the temporal width of one cycle of the electric field in the optical wavelength regime. By applying angle-resolved electron spectroscopy, the KLL Auger decay in atomic Ne was studied after excitation with few-fs X-ray (1 keV) pulses in the presence of an optical (800 nm) dressing field [1]. The experimental spectra are marked by strong interference effects caused by the coherent emission of electrons produced during one cycle of the superimposed optical dressing field, in excellent agreement with theoretical work [2].

[1] M. Meyer et al., Phys. Rev. Lett. **108**, 063007 (2012)
[2] A.K. Kazansky, N.M. Kabachnik, J.Phys.B **42**, 121002 (2009); **43**, 035601 (2010)

Controlling core hole relaxation dynamics via intense optical fields

T. Mazza,[1] K. G. Papamihail,[2] P. Radcliffe,[1] W.B. Li,[3] T. J. Kelly,[4] J. T. Costello,[4] S. Düsterer,[5] P. Lambropoulos,[2] M. Meyer[1]

[1]*European XFEL GmbH, Albert-Einstein-Ring 19, D-22761 Hamburg, Germany*
[2]*IESL-FORTH, P.O.Box 1527 and Physics Department, University of Crete, Heraklion, Crete 71110, Greece*
[3]*Institute of Precision Optical Engineering, Department of Physics, Tongji University, 1239 SiPing Road, Shanghai 200092, China*
[4]*National Center for Plasma Science and Technology and School of Physical Sciences, Dublin City University, Dublin, Ireland*
[5]*HASYLAB at DESY, Notkestraße 85, D-22607 Hamburg, Germany*

The influence of a strong optical field on the electronic relaxation of the 3d – 5p resonance in atomic Kr has been studied experimentally using intense femtosecond NIR pulses superimposed to XUV pulses from the FLASH Free Electron Laser in Hamburg.
The experiments show that the XUV-induced resonance profile undergoes a strong modification as a function of the optical intensity. The changes are observed as a shift and a broadening of the excitation spectrum. The theoretical treatment of the process demonstrates the importance of strongly time-dependent dynamics as the origin of the observed phenomena, resulting in the ponderomotive shift of the resonance position as well as in a competition between resonant and normal Auger decay after ionization of the excited 5p electron by the optical laser.

The results emphasize the possibility to modify and control the ionization dynamics by the external NIR field on a femtosecond timescale. In particular, they demonstrate the ability to control the XUV absorption cross-section of atoms at a given photon energy via the intensity of the superimposed optical laser, changing an opaque to a transparent medium and vice versa. Moreover it is possible to select the final ionic state by controlling the relaxation of the resonant core hole state through optical laser ionization of the excited 5p electrons. The detailed analysis of the experimental data and the comparison to the theoretical results will be presented at the workshop.

Linear dichroism in short-pulse two-color XUV+IR multiphoton ionization of atoms

N.M. Kabachnik[1] and A.K. Kazansky[2]

[1]*Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Leninskie Gory, Moscow, 119234, Russia*

[2]*Donostia International Physics Centre (DIPC), E-20018 San-Sebastian/Donostia, Spain*

We consider theoretically the photoionization of atoms by a short extreme ultraviolet (XUV) pulse in the presence of a strong field of the infrared (IR) laser pulse. In this case in the photoelectron spectrum, beside the usual photoline, several sidebands appear separated by the energy interval equal to the IR field quanta. If XUV and IR beams are collinear and both are linearly polarized, the photoelectron yield depends on the angle between their polarizations. The difference in the yield for the cases of parallel and perpendicular polarizations of the XUV and IR fields is usually called linear dichroism. Using a simple model of the ionization process, based on the strong-field approximation, we calculated the linear dichroism for XUV+IR photoionization of He. We have also obtained a simple analytical expression for the linear dichroism. The results of calculations show that the linear dichroism is rather large and strongly depends on the intensity of the IR laser.

Manifestation of discrete and autoionizing states in sequential atomic ionization by few XUV photons

E.V. Gryzlova[1], A.N. Grum-Grzhimailo[1], N.M. Kabachnik[1,2], S.I. Strakhova[1]

[1] *Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Leninskie Gory, Moscow, 119234, Russia*

[2] *European XFEL GmbH, Albert-Einstein-Ring, Hamburg, 22761, Germany*

Investigation of ionic spectra in photoabsorption processes has been restricted because of problems with creating ionic targets with high enough density. With the development of free electron laser (FEL) technique, observation of radiative excitation of discrete and autoionizing ionic states becomes possible by photoelectron spectroscopic methods [1-4]. For the photon energies between first and second ionization thresholds, the following main transitions take place in a noble gas target:

(1) Atomic ionization
$$A(np^6) + \gamma_1 \rightarrow A^+(np^5) + e_1\ell_1$$

(2) Ionic excitation
$$A^+(np^5) + \gamma_2 \rightarrow A^{+*}(np^4n'\ell')$$

(3) Ionization of excited ionic states
$$A^{+*}(np^4n'\ell') + \gamma_3 \rightarrow A^{++}(np^4) + e_2\ell_2$$

Excitation of autoionizing ionic states
$$A^{+*}(np^4n'\ell') + \gamma_3 \rightarrow A^{+**}(np^3n'\ell'n''\ell'')$$

(4) Decay of autoionizing ionic state
$$A^{+**}(np^3n'\ell'n''\ell'') \rightarrow A^{++}(np^4) + e_2\ell_2$$

The first step, i.e. atomic photoionization (1), is followed by photoexcitation of the ion (2). The excited ion is afterwards either directly ionized (3, left) or ionized via excitation (3, right) and decay (4) of an autoionizing state (AIS), producing the doubly charged ion. In the first case ('left'), configuration, term and acquired polarization of the excited state determine the photoelectron e_2 angular distribution. In the second case ('right'), excited state(s) serves as a kind of filter for possible excitations of AISs. Polarization of the AISs determines angular distribution of the electron e_2 and crucially affects ionization branching into different terms of the residual ion $A^{++}(np^4)$.

Experiments performed at SPring-8 with Ar at photon energies ~21 eV and ~24 eV proved that the both mechanisms, 'left' [3] and 'right' [1,2,4], take place, although interpretation of the results is difficult because of high density of discrete and autoionizing states involved in the process. The main problem in explaining these experiments is uncertainties in the Ar^+ spectrum. One may predict that investigations at lower photon energies will give clearer picture. At the energies below 20 eV there are only a few efficiently excited discrete states $Ar^{+*}(3p^4n'\ell')$: $3p^4(^3P)4s\ ^2P$ (17.2 eV), $3p^4(^3P)3d\ ^2P$ (18.0 eV), $3p^4(^1PD)4s\ ^2D$ (18.4 eV), $3p^4(^3P)3d\ ^2F$ (18.5 eV), $3p^4(^3P)3d\ ^2D$ (18.7 eV). All these excitations are potentially followed by excitation of AISs. The new experiments could verify spectroscopic models for Ar^+. The report overviews joined experimental and theoretical investigation of argon three-photon triple ionization at photon energies ~21 eV and 24 eV, together with theoretical predictions for lower energy region, where interpretation is supposed to be more transparent.

The research is supported by the Russian President grant MK-6509.2012.2 and RFBR grant 12-02-01123.

[1] Y. Hikosaka et al, Phys. Rev. Lett. **105**, 133001 (2010).
[2] N. Miyauchi et al, J. Phys. B **44**, 071001 (2011).
[3] H. Fukuzawa et al, J. Phys. B: At. Mol. Opt. Phys. **43,** 111001 (2010).
[4] E.V. Gryzlova et al, Phys. Rev. A **84**, 063405 (2011)

Non-resonant transitions in sequential three-photon double atomic photoionization of noble gases in the XUV

A.S. Bityutskaya[1,2], E.V. Gryzlova[2], A.N. Grum-Grzhimailo[2], S.I. Strakhova[2]

[1]*Faculty of Physics, Lomonosov Moscow State University, Leninskie Gory, Moscow, 119234, Russia*
[2]*Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Leninskie Gory, Moscow, 119234, Russia*

Sequential three-photon double non-resonant ionization (STDNI) of atoms is one of the phenomena, which became observable experimentally with the advent of FELs. The process proceeds in two steps. First, singly charged intermediate ion is created when the neutral atom absorbs one photon. Second, further double-photon non-resonant ionization of the intermediate ion leads to final double-charged ion. The complicated shapes of the photoelectron angular distributions (PADs) generated by the three linearly polarized along the z axis photons give information on the dynamics of this nonlinear process.

Our theoretical approach to the angular patterns for the above-mentioned process is a development of the successful formalism used in the case of the two-photon sequential double ionization [1]. A general expression is derived for the PADs in terms of the density matrix and statistical tensors in the dipole approximation. The non-resonant second step of the STDNI brings new features in comparison with the recently considered case of resonant second step [2]. Within the second-order perturbation theory, the radial amplitude of two-photon non-resonant transitions includes a summation over the whole spectrum of allowed bound and continuum states. The most difficult problem is accounting for atomic transitions in continuum (free-free transitions), which we solved using a suitable technique [3]. Particular calculations are performed for the STDNI of Ne at the photon energies 21-27 eV.

The research is supported by the Russian President grant MK-6509.2012.2 and RFBR grant 12-02-01123.

[1] S. Fritzsche, A.N. Grum-Grzhimailo, E.V. Gryzlova and N.M. Kabachnik, J. Phys. B: At. Mol. Opt. Phys. **41,** 165601 (2008).
[2] H. Fukuzawa et al, J. Phys. B: At. Mol. Opt. Phys. **43**, 111001 (2010).
[3] T. Mercouris, Y. Komninos, S. Dionissopoulou, and C.A. Nicolaides, Phys. Rev. A **50,** 4109 (1994).

Beyond the dipole approximation in two-photon ionization at FELs

A.N. Grum-Grzhimailo[1], E.V. Gryzlova[1], A.S. Bityutskaya[1,2], S.I. Strakhova[1]

[1]*Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Leninskie Gory, Moscow, 119234, Russia*

[2]*Faculty of Physics, Lomonosov Moscow State University, Leninskie Gory, Moscow, 119234, Russia*

It is known that already at photon energies of a few hundreds eV, the photoelectron angular distribution (PAD) in atomic single-photon ionization can be affected significantly by interference between electric dipole (E1) and electric quadrupole (E2) amplitudes. Thus, nondipole effects should be present also in the XUV/X-ray nonlinear atomic processes, accessible with FELs. Up to date, the study of nondipole nonlinear phenomena in atomic multi-photon ionization is restricted to a special case of resonant ionization by equivalent photons in the optical regime, when the photon frequency is in resonance with a discrete quadrupole E2 transition. Furthermore, the vast majority of nonlinear photoionization studies consider one-colour ionization with photons of equivalent frequencies and states of polarization.

In our theoretical developments we focus on two-photon two-colour ionization within the lowest-order nondipole corrections. In this case, the interaction of one of the photons with the atom can be described within the electric dipole E1 approximation, while for the other photon accounting for the lowest-order nondipole corrections is needed. This situation is realized for pump-probe experiments with combined XUV/X-ray and optical laser beams and for sequential two-photon double ionization when the electrons are not detected in coincidence. Considering collinear beams and unpolarized initial atomic states, general parameterizations of the PADs and dichroism in the angular distributions have been derived for circularly and linearly polarized radiation. For parallel polarization directions of the collinear linearly polarized beams, the PAD, within the first order nondipole corrections, takes the form

$$W(\Theta,\Phi) = W_0\,[1 + \beta_2 P_2(\cos\Theta) + \beta_4 P_4(\cos\Theta) + (\delta + \gamma_2\cos^2\Theta + \gamma_4\cos^4\Theta)\,\sin\Theta\cos\Phi]$$

where the angles of the electron emission Θ and Φ are counted from the directions of the polarization and the momentum of the photons, respectively, $P_n(x)$ are the Legendre polynomials and β_n, γ_n, δ are the dynamical parameters. The first three terms correspond to the pure dipole contribution; the last three terms give the first-order nondipole corrections. The last term with γ_4 is a specific nondipole correction for two-photon ionization. Fig.1 shows some of our results for sequential two-photon double ionization (TPDI) of Ne:

1 step $\gamma + Ne(2p^6) \rightarrow Ne^+(2p^5) + e_1$;

2 step $\gamma + Ne^+(2p^5) \rightarrow Ne^{++}(2p^{4\,2S+1}L) + e_2$

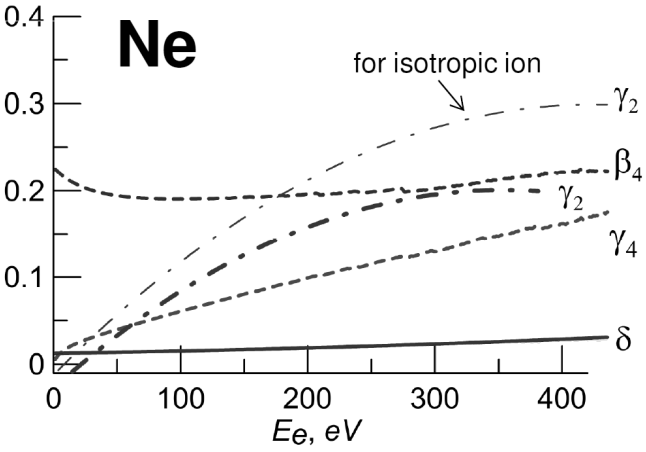


Fig. 1. Dynamic parameters β_4, γ_2, γ_4, δ of PAD in sequential TPDI of Ne into the final state $Ne^{++}(2p^{4\,1}S)$ as functions of energy of the second-step electron e_2.

The research is supported by the Russian President grant MK-6509.2012.2 and RFBR grant 12-02-01123.

Non-dipole effects in (γ, 2e) processes caused by photon momentum

A.G. Galstyan[1] , O. Chuluunbaatar[2] , Yu.V. Popov[3], and B. Piraux[4]

[1] *Physics Faculty, Moscow State University, Moscow, Russia*
[2] *Joint Institute for Nuclear Research, Dubna, Russia*
[3] *Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow, Russia*
[4] *Institute of Condensed Matter and Nanosciences, Universite catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium*

In dipole approximation, vector potential $\vec{A}(\vec{r},t)$ is considered as independent on $\vec{r}$ at characteristic atomic distances of interaction. However, for very high frequencies, the vector potential may vary significantly over typical atomic distances. In these conditions, it is important to take explicitly into account the dependence of $\vec{A}$ on the position vector $\vec{r}$ in its the simplest form $\vec{A} \sim \vec{e}[\exp(i\vec{k}\vec{r} - i\omega t) + \text{c.c.}]$ with polarization $\vec{e}$ and photon momentum $\vec{k}, \vec{k} \perp \vec{e}$.

We study the influence of the photon momentum $\vec{k}$ on triple differential cross section (TDCS) of (γ, 2e) processes. Such effects were first considered by Amusia *et al* in [1], and recently were found experimentally [2]. These effects are very weak because of small magnitude of the photon momentum and can be obtained only in special kinematical conditions such as back-to-back emission of electrons with equal energy sharing, where the dipole approximation gives zero of TDCS.

Rather unexpectedly, absolute TDCS dependence on photon energy reaches its maximum at low energies. Indeed, this effect appears only when we take account electron correlations in the double electron final state wave function. The dependence of the maximum of TDCS for different light K-ions on the charge of nucleus was also studied and corresponding electron energies were obtained [3].

[1] M. Ya. Amusia et al., J. Phys. B **8**, 1248 (1975).
[2] M. S. Schoeffler et al., Abstracts of XXVII ICPEAC, Th132 (2011)
[3] A. G. Galstyan et al., Phys. Rev. A **85**, 023418 (2012)

Poster session

The variable polarization XUV beamline P04 at PETRA III

Leif Glaser, Sascha Deinert, Markus Ilchen, Frank Scholz, Jörn Seltmann, Peter Walter and Jens Viefhaus

Deutsches Elektronen Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

The Variable Polarization XUV beamline P04 at PETRA III, which is presently under commissioning, will enable new classes of experiments with soft x-rays in the fields of gas phase physics, magnetic spectroscopy, high resolution photoelectron spectroscopy, surface chemistry, soft x-ray diffraction and holography. The unique characteristics of this beamline are an exceptionally high photon flux – up to several 10E+12 photons per second – in a very small bandpass (resolving power exceeds 10,000) as well as variable polarization properties over a very wide energy range (200-3000 eV) using only the first harmonic of an APPLE-2-type undulator. Due to the very low emittance of the PETRA III storage ring the radiation of the beamline is practically coherence limited in whole photon energy range except for the horizontal source size (300 µm FWHM). Results of the ongoing commissioning phase including the associated university projects funded via the BMBF "Verbundforschung" will be presented.

Poster session

Direct-Monte-Carlo-Simulations of Gas Dynamics and Properties for Synchrotron Radiation and Free Electron Laser Applications

Jörn Seltmann, Sascha Deinert, Leif Glaser, Markus Ilchen, Frank Scholz, Peter Walter, and Jens Viefhaus

Deutsches Elektronen Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

XUV/VUV spectroscopic measurements involving atoms and molecules such as gas phase photoelectron spectroscopy experiments typically employ a gas injection with molecular flow into a vacuum environment. In these experiments special requirements have to be fulfilled, such as a small interaction region with a high gas density compatible with the high vacuum environment. In our work a direct Monte-Carlo-Simulation software package [1] was utilized to optimize the pressure in the interaction region relative to the total pressure in the vacuum chamber. Additionally we have validated the efficiency of multi-capillary gas inlets as proposed by Seccombe et al. [2]. We present results of different simulations and a comparison of simulation and measurements using different setups relevant for gas phase experiments in combination with synchrotron radiation or free electron lasers. In some applications it is necessary to maintain a pressure difference between the experiment and the beamline. This can be achieved by using a differential pumping section employing a high impedance connection together with additional pumping with the great advantage over foils that the photon flux and wave front is not disturbed. Using the direct Monte-Carlo-Simulation tool it is possible to optimize the design of the differential pumping system with respect to gas flow dynamics and minimized pump requirements for a given tolerable gas flux into the beamline.

[1] G.A. Bird; “Molecular Gas Dynamics and the Direct Simulation of Gas Flows”, Clarendon Press, Oxford 1994

[2] D.P. Seccombe, Collins, Reddish; Rev. Sci. Instr. **72,** 2550 (2001)

Poster session

On application of STJ detectors in synchrotron-based X-ray spectroscopy

V. A. Andrianov[1], S.N. Ryazantsev[2]

[1]*Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Leninskie Gory, Moscow, 119234, Russia*
[2]*Faculty of Physics, Lomonosov Moscow State University, Leninskie Gory, Moscow, 119234, Russia*

At present, an active research is ongoing in the field of development of new detectors of X-ray radiation and optical radiation on the basis of superconducting tunneling junctions (STJs) [1]. In these detectors energy is absorbed in a superconducting metallic electrode. The energy breaks Cooper pairs and the excess electronic excitations called quasi-particles are created. These quasi-particles cause amplification of tunneling current, which, in fact, forms STJ detector signal.

Since the average energy to create an excess charge carrier scales with the energy gap Δ, which is of the order of ~1 meV and thus roughly a factor ~1000 smaller than the gap in semiconductors, STJ detectors can have 30 times better energy resolution than Si or Ge detectors. The theoretically expected energy resolution for detectors with Nb electrodes is ~ 1.6 eV for 100 eV, ~5 eV for 1 keV and ~13 eV for the X-ray line at 6 keV [1].

In this report applications of STJ detectors in the energy range from 100 eV to 1 keV will be discussed. This energy range corresponds to the soft X-rays of light elements. Two types of STJ-detectors, symmetric detectors and detectors with «killed» electrode are considered. Both of them have their own advantages. In the symmetric detector, the signal can be increased by multiple tunneling processes [1]. The detectors with killed electrode have a short duration of the signals [2].

The perspectives of STJ detector usage in synchrotron-based research are considered. The high energy resolution of STJ devices makes them competitive for the EXAFS and XANES spectroscopy of light elements, especially in case of a small concentration in the samples.

[1] P. Lerch, A. Zender, Quantum Giaever Detectors in Cryogenic Particle Detectors. Topics in Applied Physics. Christian Enss (Editor), Springer **99**, 217 (2005)
[2] V. A. Andrianov, V. P. Gorkov, V. P. Koshelets, L. V. Filippenko, Semiconductors **41**, 215 (2007).

Poster session

LASER-ASSISTED ELECTRON-IMPACT IONIZATION OF ATOMS AT HIGH IMPACT ENERGY AND LARGE MOMENTUM TRANSFER

Andrey A. Bulychev[1], Konstantin A. Kouzakov[1,2], Yuri V. Popov[2], and Masahiko Takahashi[3]

[1]*Faculty of Physics, Lomonosov Moscow State University, Moscow 119234, Russia*
[2]*Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow 119234, Russia*
[3]*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan*

We report on a theoretical consideration [1,2] of the (*e*,2*e*) method at high impact energy and large momentum transfer, which is often referred to as the electron momentum spectroscopy (EMS) [3], in the presence of a laser field. One of the main purposes of our study is to examine the potential of EMS for investigating the laser effect on the electron momentum density of atomic systems. The laser electric field amplitude is supposed to be much weaker than the intraatomic field, and the laser frequency well below the frequency of the transition from the ground to the first excited target state. We present and analyze the results of numerical calculations of the triple differential cross sections (or the so-called momentum profiles) for the laser-assisted (*e*,2*e*) processes on atomic hydrogen and helium in symmetric noncoplanar EMS kinematics.

[1] K.A. Kouzakov, Yu.V. Popov, and M. Takahashi, *Phys. Rev. A* **82**, 023410 (2010)
[2] A.A. Bulychev, K.A. Kouzakov, and Yu.V. Popov, *Phys. Lett. A* **376**, 484 (2012)
[3] E. Weigold and I.E. McCarthy, *Electron Momentum Spectroscopy* (Kluwer, New York, 1999).

Poster session

Ionization of atomic and trapped hydrogen by intense short VUV pulses

M.N. Khaerdinov, A.N. Grum-Grzhimailo, E.V. Gryzlova, and S.I. Strakhova

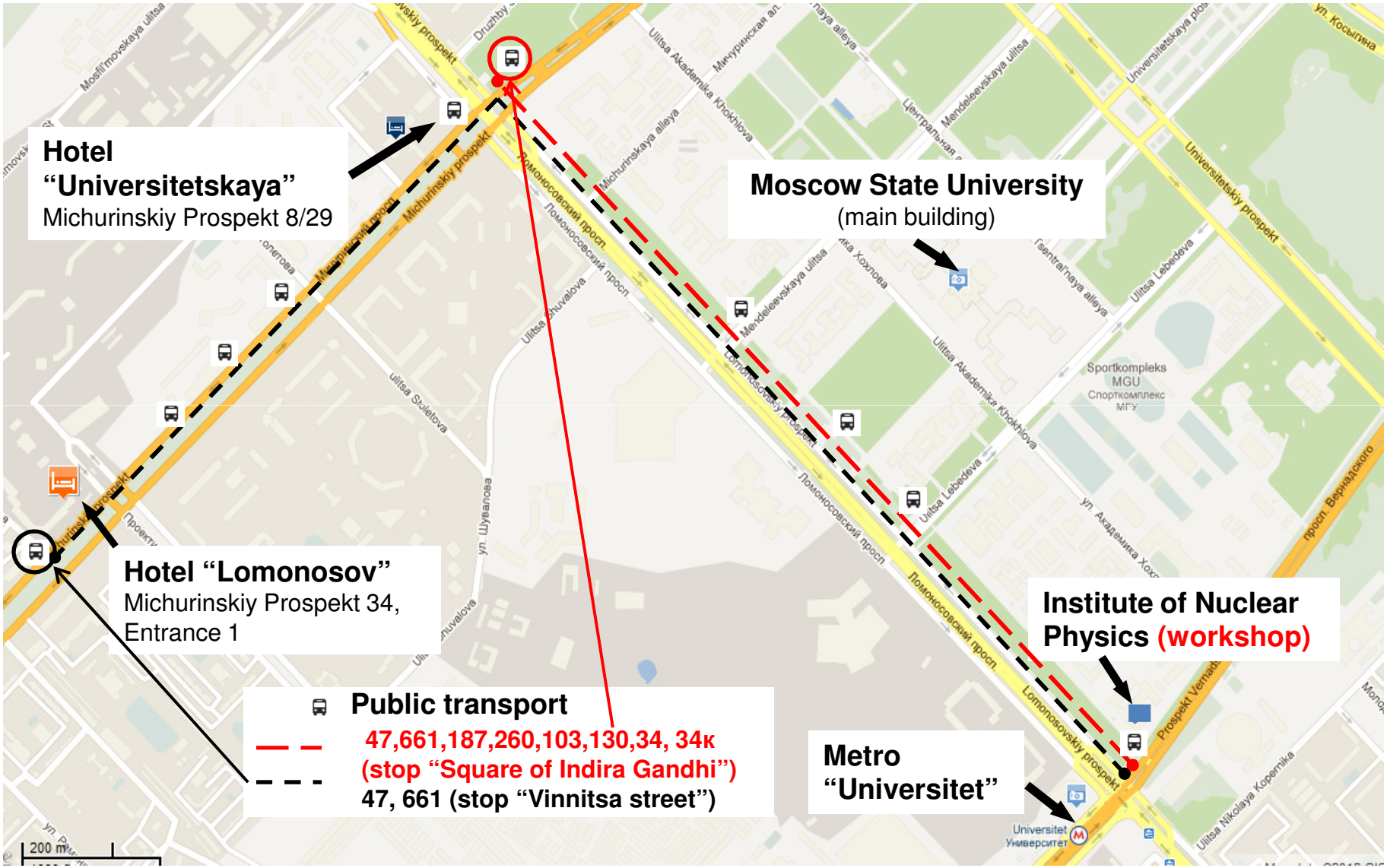
Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Leninskie Gory, Moscow, 119234, Russia

As a further application of the matrix iteration method (MIM) for numerical solution of the time-dependent Schrödinger equation (TDSE) [1-3], we calculated photoionization of the hydrogen atom in two special cases: (a) isolated hydrogen atom, energy of photons 0.375 a.u. in resonance with the 1s→2p transition; (b) hydrogen atom encapsulated into the fullerene [4].

In the first case, we took the ~16.2 fs pulse (40 optical cycles) with intensity of $4 \cdot 10^{14}$ W/cm^2, when strong disagreement between three various calculations occurs: two numerical TDSE results and model calculations with separable potential [5] give essentially different photoelectron spectra for the electron energies above ~60 eV. Our calculations by the MIM code, especially suited for high radiation intensities, show the high-energy 'shoulder' in the photoelectron spectrum, which is similar to [5], but without the above-threshold ionization (ATI) structures, which die at these energies.

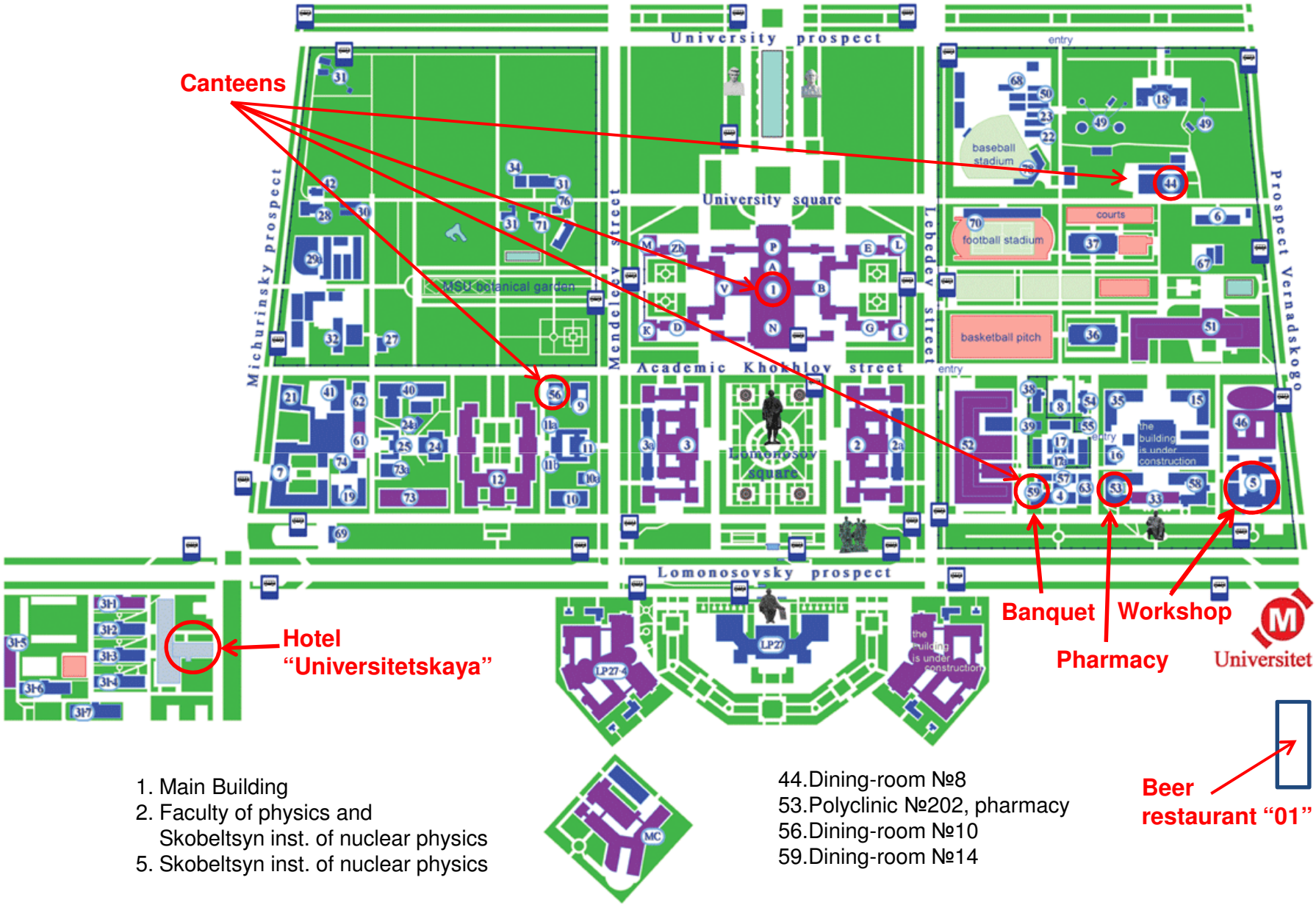
The influence of the fullerene C_{36} and C_{60} confining potentials on the ionization of a trapped hydrogen atom by a strong VUV femtosecond pulse was studied. The confinement oscillations in the intensity of the main photoelectron line for ionization from the well localized 1s state disappear with increasing strength of the radiation field. The influence of the cage is larger for the angular distribution parameters of the photoelectrons in the above-threshold ionization (ATI) peak(s), due to switching on other than εp interfering partial waves. Ionization from the 'hybrid-like' 2s state is much more sensitive to the cage potential than ionization from the 1s state; a strong influence of the cage on the intensities and angular distributions of photoelectrons from the 2s state goes far beyond the weak-field domain and persists for both the main and the ATI photoelectron lines. Although the calculations were performed for atomic hydrogen, we believe that some of the general trends hold true for other trapped atoms.

[1] A.N. Grum-Grzhimailo et al, Phys. Rev. A **81**, 043408 (2010)
[2] M. Schuricke et al, Phys. Rev. A **83**, 023413 (2011)
[3] M.G. Pullen et al, Opt. Lett. 36, 3660 (2011)
[4] A.N. Grum-Grzhimailo, E.V. Gryzlova and S.I. Strakhova J. Phys. B: At. Mol. Opt. Phys. **44**, 235005 (2011)
[5] H.M. Tetchou Nganso et al, Phys. Rev. A **83**, 013401 (2011)


Hotel
“Universitetskaya”
Michurinskiy Prospekt 8/29
Moscow State University
(main building)
Hotel “Lomonosov”
Michurinskiy Prospekt 34,
Entrance 1
Institute of Nuclear
Physics (workshop)
Public transport
47,661,187,260,103,130,34, 34к
(stop “Square of Indira Gandhi”)
47, 661 (stop “Vinnitsa street”)
Metro
“Universitet”
Michurinskiy prospekt
Lomonosovskiy prospekt
Universitetskiy prospekt
Mendeleevskaya ulitsa
Ulitsa Akademika Khokhlova
Ulitsa Lebedeva
Michurinskaya alleya
Sportkompleks
MGU
Universitet
200 m

To get to Lomonosov Moscow State University, Hotel Universitetskaya and Hotel Lomonosov get off at metro station "Universitet"

The scheme of an arrangement of MSU buildings on Leninskiye Gory



1. Main Building
2. Faculty of physics and Skobeltsyn inst. of nuclear physics
5. Skobeltsyn inst. of nuclear physics

44. Dining-room №8
53. Polyclinic №202, pharmacy
56. Dining-room №10
59. Dining-room №14