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From the Editor's Desk

Natural science has benefited immensely from developments in computing technologies. Today, it would be impossible to find research papers in physics journals which have not used computers in one way or other. The research work itself, preparation of the manuscript, submitting the manuscript, refereeing, typesetting, printing and posting; - all require computers. Not to forget, one may need a computer even for reading the published research papers! The buggy software and interface problems are numerous, despite these, the overall impact is very positive. Designing or controlling advanced and complex experimental facilities are made easier with computers. Perhaps, the advances in computer technology are a boon for theoretical physicists who study many-body systems like atom or molecules. Solving theoretical problems of increasing complexities have become possible with the continuing reign of Moore's law, according to which, every twenty four months, the density of transistors etched on silicon wafers doubles. This translates into higher raw computing power and offers the possibility to work on more complex research projects. May the Moore's law hold true for years to come. The downside of all these is coming to be appreciated, but the odds are heavily loaded in favour of wider use of computers.

Huge amounts of data and computational power lies distributed over the globe. The advances in networking make it plausible that these data and computational power be married without their being in the same place. The article on *e-Science* in this issue focuses on this manner of doing Science using global data and efficiently networked computational resources.

This newsletter contains 17 abstracts *(a record so far!)*, two synopses of Thesis *(for the first time)* and also some useful information on Royal Society (UK) grants. A few deadlines are close, however ambitious ones can still make it.

Also, we enter the third year of this activity . . .

K. P. Subramanian, Editor **Dilip Angom, Guest Editor**

Contents of this volume:

Abstracts

1. Influence of Young-type interference on the forward-backward asymmetry in electron emission from H_2 in collisions with 80-MeV bare C ions

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We use the forward-backward angular asymmetry in the electron emission cross sections in fast ion impact ionization of H_2 as a probe of the inversion symmetric coherence in homonuclear diatomic molecules. The electron energy dependence of the asymmetry parameter for H_2 exhibits oscillatory structure due to Young-type interference in contrast to atomic targets such as He. The asymmetry parameter technique provides a self-normalized method to reveal the interference oscillation independent of theoretical models and complementary measurements on atomic H target.

Phys. Rev. A **74**, 060701(R) (2006): Rapid. Comm.

2. Infrared spectra of C_2H_2 under jet-cooled and *para*-H_2 matrix conditions

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In spectra of jet-cooled C_2H_2 recorded with an FTIR spectrometer, the ν_5, $\nu_4+\nu_5$, ν_3 and $\nu_2+\nu_4+\nu_5$ bands all exhibit an intensity distribution corresponding to ~6 K for rotation, with no evidence of nuclear spin conversion. Spectra of C_2H_2 isolated in solid p-H_2 show no evidence of rotation of C_2H_2. The strong interaction between ν_3 and $\nu_2+\nu_4+\nu_5$ in the gas phase is diminished in solid p-H_2. Lines associated with dimer, trimer and tetramer of C_2H_2 are identified. Spectral features characteristic of solid state acetylene are observed under jet-cooled conditions.

Chem. Phys. Lett. **435** (2007) 247

3. Theoretical studies of the $6s^2S_{1/2} \rightarrow 5d^2D_{3/2}$ parity non-conserving transition amplitude in Ba^+ and associated properties

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It is widely believed that the standard model (SM) of particle physics is just an intermediate step in understanding the properties of the elementary physics in nature and the interactions between them. Over the last twenty years, studies of the parity non-conservation in atomic systems based on non-accelerator methods have made remarkable progress. An experiment to measure parity non-conservation in singly ionized barium has been proposed as an independent test of the Standard Model. We have employed the relativistic coupled-cluster theory to calculate the parity non-conserving $6s\ ^2S_{1/2} \rightarrow 5d\ ^2D_{3/2}$ transition amplitude and associated properties. We have also shown contributions from various intermediate states which play a significant role in the determination of this transition amplitude.

Phys. Rev. A **75**, 032507 (2007)

4. Laser frequency offset locking using electromagnetically induced transparency

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We have used an electromagnetically induced

transparency resonance in rubidium as a dispersive reference to lock the relative frequency of two lasers to the atomic ground-state hyperfine splitting. The beat frequency between the two lasers directly generates a microwave signal at 3.036 GHz (^{85}Rb) or 6.835 GHz (^{87}Rb). High bandwidth (600 kHz) feedback was achieved with only low-frequency (10 MHz) electronics using the frequency modulation sideband method. The spectral width of the microwave beat frequency was reduced to less than 1 kHz. The technique offers a convenient and low-cost method suitable for many topical two-frequency experiments, including coherent population trapping, slow light, lasing without inversion, and Raman sideband cooling.

Phys. Rev. A **74**, 064701 (2006)

5. Experiments on the reflection of cold atoms from magnetic thin films: From atom optics to measurement of short-range forces

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We report the results from a series of experiments in which ferromagnetic thin films were used as atom mirrors for laser-cooled rubidium atoms released from a magneto-optical trap. The thin films were made of cobalt and lanthanum calcium manganite (LCMO) with thicknesses between 20 and 300 nm. The magnetic domains in these thin films have a periodic structure where the spatial period is of the order of the thickness of the film, and the field decays exponentially above the film over a length scale comparable to the domain size. Thus, the neutral atoms reflect off these films from distances comparable to the thickness of the film, resulting in modification of the reflectivity due to the competition between the repulsive magnetic force and the attractive short-range forces such as van der Waals and Casimir forces. The smoothness of the atom mirror is also modified due to the proximity of the magnetic domains. The reflectivity is sensitive to the domain structure and size, which can be modified in LCMO by applying a modest external magnetic field. In this paper, we discuss the evaluation of the thin films as magnetic mirrors for atom optics, and the measurement of the van der Waals force with an accuracy of about 15%, using cobalt thin films. We also discuss some preliminary results on the temperature-dependent reflectivity for atoms near the ferromagnetic transition at 250 K in the LCMO film, and on the domain dynamics and relaxation.

Eur. Phys. J. D **42**, 287-298 (2007)

6. Quantum information cannot be completely hidden in correlations: Implications for the black-hole information paradox

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Can quantum information theory shed light on black hole evaporation? By entangling the in-fallen matter with an external system we show that the black-hole information paradox becomes more severe, even for cosmologically sized black holes. We rule out the possibility that the information about the in-fallen matter might hide in correlations between the Hawking radiation and the internal states of the black hole. As a consequence, either unitarity or Hawking's semi-classical predictions must break down. Any resolution of the black-hole information crisis must elucidate one of these possibilities.

Phys. Rev. Lett. **98**, 080502 (2007)

7. Coplanar doubly symmetric (*e*,2*e*) process on sodium and potassium

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We have used the distorted-wave Born approximation method to analyze the recently reported (*e*,2*e*) experimental results on sodium and potassium atoms in doubly symmetric geometry at excess energies of 6, 10, 15, 20, 30, 40, 50 and 60 eV. Post-collision interaction is included through an angle-dependent effective charge model using two different approximations. Our theoretical results are found to qualitatively reproduce the reported experimental data.

Phys. Rev. A **74**, 064701 (2006)

8. Angular distribution of Au and U *L* x rays induced by 22.6 keV photons

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The angular distribution of the L x-rayflourescent lines from Au and U induced by 22.6-keV x rays from a ^{109}Cd has been measured. A Si(Li) detector having a resolution of 160 eV at 5.90 keV was used to detect these L lines over the angular range of $70^\circ - 150^\circ$. No strong anisotropy was observed as mentioned by some groups. In the case of Au, a maximum anisotropy of 5% was observed while for U it was within experimental errors (2%). From the angular distribution of $L1$ line of Au, the alignment parameter was obtained and its value was found to be 0.10 ± 0.14.

Phys. Rev. A **75** 022901 (2007)

9. Significant longer-term periodicities in the proxy record of the Indian monsoon rainfall

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Recently stable carbon and oxygen isotope ratios (denoted by δ^{18}O and δ^{13}C respectively, proxies for monsoon rainfall) of the last 331 years from an annually laminated speleothem were measured. The time-series analysis of the data using Fast Fourier Transform (FFT) and the Maximum Likelihood Analyses (MLA) reveals significant power in several periods that have a likely solar origin e.g. 132, 21, 18, and 2.4 years. These cycles are non-stationary in nature. Using wavelet analysis we find that the ∼21-year period is strong during 1850 to 1920 A.D. Between 1780 and 1920 A.D., low rainfall intervals are concurrent with low solar activity. However, this behavior breaks down for the older periods. In the δ^{13}C periodogram, additional significant periods appear viz. ∼59, ∼8, ∼6.5 and ∼3 years: these could have originated from solar variations and/or changes in the biological degradation of soil carbon. Surprisingly, while the low power solar cycles (viz. ∼22 yr and ∼2.4 yr) are seen in the δ^{18}O and δ^{13}C spectra with the ∼21 yr cycle dominating, the stronger ∼11 year cycle is only weakly represented in the proxy record, confirming earlier findings based on amore limited data set.

New Astronomy (in press, 2007)

10. Dynamic multiple scattering, frequency shift and possible effects on quasars astronomy

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The shifting of spectral lines due to induced correlation effect, discovered first by Wolf for the single scattering case which mimics the Doppler mechanism has been extended and developed further by the present authors to study the behavior of spectral lines in the case of multiple scattering and observed shifting, as well as broadening of the spectrum. We have explored Dynamic Multiple Scattering(DMS) theory for explaining anomalous redshifts in quasars. Our recent work, based on the statistical analysis of the Véron-Cetty data(2003) supports that quasar redshifts fit the overall Hubble expansion law, as in the case of galaxies, for $z < 0.295$ but not for higher redshifts, indicating clearly the inadequacy of the Doppler effect as the sole mechanism in explaining the redshifts for high redshift quasars($z > 0.295$). We found that the redshift posseses an additive,"discordant" component due to frequency shifting from the correlation induced mechanism which increases gradually for $0.295 < z < 3.0$, however, appearing to follow the evolutionary picture of the universe with absolute dependence on the physical characteristics i.e., environmental aspects of the relevant sources through which the light rays pass, after being multiply scattered. According our framework, as the environment around sources is diverse, subject to the age of the universe, it determines the amount of multiple scattering effect, probably, without additional additive effects for higher values i.e., for redshifts $z > 0.295$. The recent observational data on redshift z versus apparent magnitude(m) (Hubble like relation) are found to be in good agreement, considering suitable values of the induced correlation parameters. This resolution of the paradox of quasar redshifts is much more appealing and in a sense, more mainstream physics than either assigning redshift entirely to the Doppler effect or inventing a new, often unknown, physical mechanism. Our analysis indicates the importance of local environmental aspects of relevance (recent observations of molecular gases, the plasma like environment, evolution of the hydrogen content with epoch etc.) around quasars, especially for the higher redshift limits. Our work opens possible new vistas in quasar astronomy as well as for cosmological models of the universe.

Int. J. Mod. Phys. D (Submitted, 2007)

11. Correlation-induced spectral changes due to

multiple scattering in the spatio-temporally fluctuating random medium: Possible implications on Hubble relation and quasar redshift anomaly

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A framework of multiple scattering has been developed, by the authors and other collaborators, considering the medium as anisotropic [first discovered in case of single scattering by Emil wolf in 1987, thereafter called as the Wolf effect], consisting of thin multiple layers. This mechanism deals with correlation-induced spectral changes in a model scattering medium with spatio-temporally fluctuating dielectric response function which produces shifts of spectral lines imitating the Doppler effect in its main features. The possible relevance of this effect is far reaching in case of explaining the discrepancies observed in some quasar spectra besides other cosmological aspects like redshift measurements, Hubble flow etc. From the statistical analysis of the Véron-Cetty catalogue for quasar(2006) and SDSS(2005), quasars are shown to fit the overall Hubble expansion law, like galaxies but only for the low values of redshift(z< 0.3) after which nonlinearity are observed. The mechanism, proposed in this paper, starts manifesting itself nearly at z= 0.3, increase up to z <2.995. Simulation has been carried out to explain this trend, considering suitable values(from experiments) of the induced correlation parameters. The results clearly produce an envelope where the huge spread observed in the redshifts of quasars can easily be explained. This points to the importance of the effect due to the intrinsic physical properties of local environment around quasars, particularly when the limit of high redshift is approached. This resolution of the paradox of quasar redshift is much more appealing and in a sense more mainstream physics than either assigning redshift entirely to the Doppler effect or inventing a new, often unknown, physical mechanisms.

Int. J. Mod. Phys. D (Submitted, 2007)

12. Reliable measurement of the Li-like $^{48}_{22}$Ti 1s2s2p $^4P^0_{5/2}$ level lifetime by beam-foil and beam-two-foil experiments

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We have determined the lifetime $^{48}_{22}$Ti 1s2s2p $^4P^0_{5/2}$ of the Li-like level (210.5±13.5 ps) using data from its x-ray decay channel through beam single- and two-foil experiments, coupled to a multi-component iterative growth and decay analysis. Theoretical lifetime estimates for this zero-nuclear spin ion lies within the uncertainty range of our experimental results, indicating that blending contributions to this level from the He-like 1s2p $^3P^0_2$ and 1s2s $^3S^0_1$ levels are eliminated within the current approach. A previously reported discrepancy between experimental and theoretical 1s2s2p $^4P^0_{5/2}$ level lifetimes in $^{51}_{23}$V may, as a result, be attributed to hyperfine quenching.

Phys. Rev. A **73** 032509 (2006)

13. Beam-single and beam-two-foil experimental facility to study physics of highly charged ions

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A facility for lifetime measurement of metastable states in highly charged ions using the beam-foil technique with a single-foil and a two-foil target has been developed. In the two-foil technique, one foil moves with respect to the other and the option of varying the thickness of the fixed foil on line has been implemented. A holder with multiple foils is used as a fixed target, and moved along x, y, and θ, the angle of rotation with respect to beam direction along z axis. Using this facility, the He-like 1s2p $^3P^0_2$ and Li-like 1s2s2p 1s2s2p $^4P^0_{5/2}$ titanium lifetimes have been measured and compared with earlier values. In addition to this, the processes which occur when excited states collide with carbon foils of different thickness have also been investigated. Preliminary results suggest the scope of studying intra-shell transitions during ion-solid collision using this setup. In this paper, the setup is described in detail and representative results are briefly discussed.

Rev. Sci. Instru. **77** 033107 (2006)

14. Effect of Foil Thickness on Excited States in the Beam-foil Interactions

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The present communication reports experimental studies on the interaction mechanism of excited states, produced by fast heavy ions passing through carbon foil, with a thin carbon foil. Oscillatory structure of the lifetime spectrum of the combined peak of M1 and M2 decays in He-like Ti-ions gives a direct evidence of the transitions between 1s2p $^3P_2$ and 1s2s $^3S_1$ states on every collision.

Asian J. Chem. **18** 3260 (2006)

15. Alteration of molecular symmetry during dissociative ionisation

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Complete momentum maps of all fragments including neutrals arising from dissociative double ionisation of CCl_4 by electron impact have been obtained. The geometry of the dissociating dication is estimated from the momentum maps. The observation of Cl_2^+ in the time-of-flight mass spectrum of the fragments combined with the momentum distribution of correlated fragments provides evidence, that the geometry of the dissociating cation is significantly altered from the tetrahedral geometry of the parent neutral. These observations suggest relocation of certain atoms within the molecular ion during dissociation. The geometry of CCl_4^{2+} derived from the momentum maps is in conformity with the theoretically generated structure.

Phys. Rev. A (Rapid. Comm.) (Submitted, 2007)

16. Observation of Giant Resonance Phenomena in the Two-Step Mechanism of Electron-Xe Collision

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We report an $(e; 2e)$ binding energy spectrum of Xe obtained at an impact energy of 2.1 keV, which covers the binding energy range up to 220 eV. The result is directly compared with data from high-energy photoelectron spectroscopy. It is found that an $(e; 2e)$-specific, very broad band appears at around 120 eV, although in other energy regions the binding energy spectra by the two methods are in good agreement. The presence of such a band is revealed for the first time, which can be attributed to the second-order effects of the electron-target interaction that involves giant resonance phenomena of the Xe 4*d* electron.

Phys. Rev. Lett. **98**, 013201 (2007)

17. Designing bound states in a band as a model for a quantum network

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We provide a model of a one dimentional quantum network, in the framework of a lattice using von Neumann and Wigner's idea of bound states in a continuum. The localized states acting as qubits are created by controlled deformation of a periodic potential using supersymmetric quantum mechanics. These wave functions lie at the band edges and are defects in a lattice. We propose that these defect states, with atoms trapped in them, can be realized in an optical lattice and can act as a model for a quantum network.

AIP Conference Proceedings Vol. 864 (2006)

Theses

EXPERIMENTAL STUDIES ON PHOTON INDUCED INNER SHELL IONISATION

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Interaction of photons with matter is one of the most fundamental processes that has widely been studied so far. Although extensively investigated, there are still some areas where more accurate and reliable data are needed. One such area is the process of creation of vacancies in the inner shells of atoms and subsequent processes like emission of diagram/ nondiagram X-ray lines, transfer of vacancies from one shell to the other, re-arrangements of vacancies among the different subshells etc.

The values of the atomic parameters especially for L/M shells, show large scatter and so instead of the theoretical values of fluorescence cross sections of these shells, directly measured values are very much needed. Here, L X-ray fluorescence cross sections of Th and U have been measured at 22.6, 25.8, 29.2 and 32.9 keV. From these fluorescence data, L subshell photoionisation cross sections have been obtained and the effect of scatter of the atomic parameters on the cross section values is discussed.

A novel method of determining the value of the Coster-Kronig transition probability (f_{23}) using the K-L X-ray coincidence technique is introduced. In earlier coincidence measurements, radioactive isotopes were used as targets which was, indeed, a limitation. In the present method, an Au foil was irradiated with 88 keV γ rays from a ^{109}Cd source. The Au K and the subsequent L X-rays are then measured in coincidence and the value of f_{23} was obtained to be 0.119 ± 0.003.

When both the K and the L shells are excited by the incident photons, a large fraction of the L shell vacancies are created through the transfer of K shell vacancies. Theoretical values of these transfer probabilities are available in the literature but very few measured values are available. An X-ray tube with secondary targets has been used for the first time to measure the K to L shell vacancy transfer probability (η_{KL}) parameter for Mo, Pd and Cd. The measured values of η_{KL} are found to be in good agreement with the theoretical values and the data of others.

It is still not clear whether the emission of L X-rays after photoionisation is isotropic or not. Different groups have performed angular distribution measurements of L X-rays induced by photons. Some groups got very high angular dependence while others got either very small or no angular dependence at all. So, the angular distribution measurements of Au and U L X-rays induced by 22.6 keV photons have been performed. From this measurement, a small anisotropy $\sim 5\%$ was found for the Au L lines while for U it was almost isotropic.

It is well known that heavy ions produce simultaneous multiple ionisation in the target which gives rise to different X-ray satellite lines. In photon induced cases multiple ionisation occurs through the process of "shake up"and "shake off". As a result of multiple ionisation, satellite and hypersatellite lines are observed. An X-ray tube with a Ag anode was used to excite the K lines of Si and P from different samples. Using a crystal spectrometer, the peak positions and the intensities of Si K_α and its satellite lines from pure Si, SiO_2 and SiC compounds and the respective peak positions of P lines from $NH_4H_2PO_4$ were obtained. These results were then compared with other available data and theoretical predictions.

The results of the compositional analysis of a few samples (coins) obtained from our Energy Dispersive X-ray Fluorescence (EDXRF) set up have been compared with those from the high energy Particle Induced X-ray Emission (PIXE) facility at Hahn-Meitner Institute, Berlin and it was found that the results agree quite well with each other. With this EDXRF system, some *Hindu* and *Buddha* statues obtained from the West Bengal Archaeological Museum were analysed. Based on their elemental composition, some remarks on the origin of the statues are made.

Submitted to : Jadavpur University, Kolkata on 23 Mar 2006

COLLISION OF ELECTRON WITH ATOMS, MOLECULES AND CLUSTERS

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The atomic and molecular cross section find their applications in the various scientific and technical fields including astrophysics aeronomy, gas lasers, plasma physics, controlled thermonuclear fusion, transport properties of gases, chemical reactions and the biological science.

At low impact energy [less than about 50 eV] one is required to solve a set of coupled integro-differential equations, whose exact solution is not possible. At intermediate energies at least the distortion of the wave function of the incident electron is to be considered. Thus along with the first Born higher terms of the Born series are to be included. At impact energy greater than about ten times the ionization potential, the first Born approximation [FBA] is expected to be valid. Even in this energy range this approximation requires the continuum generalised oscillator strengths [CGOS]. In an ionization process the final channel contains two free electron and the molecules are multi-centered objects. Due to the multi-centered nature of the initial and final wave functions of the molecule, the generation of the CGOS becomes quite difficult.

Most of the theoretical calculations have combined the contributions of the soft collisions (given by Bethe cross section) with that of the hard collisions (given by the Mott cross section) in some suitable manner to obtain the total ionization cross sections [2-4]. Margreiter et al [5] combined classical binary encounter theory with the Born-Bethe approximation to generate electron-atom ionization cross sections in the energy range 20-200 eV. These cross section are then added to obtain electron-molecule ionization cross sections. Bobeldijk et al [6] have employed a geometric additivity rule to investigate electron impact ionization of the molecule for the impact energy E varying from 15 to 150 eV. Kim and Rudd have proposed binary encounter dipole [BED] and binary encounter Bethe [BEB] models for the molecule ionization cross sections due to electron impact. They included the effect of the acceleration of the incident electron by the molecule field through the binary encounter theory and referred that model as BED model. To derive their BEB model they employed a simple representation of COOS.

In 1997 Saksena et al [7] have proposed a model for the molecule ionization cross sections. They started with the plane wave Born approximation (PWBA) but included exchange and relativistic corrections. The transverse interaction through the longitudinal interaction due to unretarded Coulomb field are also included. Also, they employed a semi-phenomenological relation of Mayol and Salvat [8] which expresses CGOS in term of COOS. The use of the above relation breaks the expression of the ionization cross section into two terms and representing the Bethe term and the other Mott term. But their model has been found to under estimate the cross section at low impact energies. Khare et al have developed another model by combining the useful features of Saksena model and BEB model of Kim and Rudd. So far this model is employed to the ionization of simplest ionization of simple atom, namely hydrogen atom [9] to methane [10].

Recently Joshipura et al [11-13] have calculated the total inelastic and total ionization cross section for collisions of electron on many atomic and molecule targets. Their calculation proceeds through a complex energy-dependent potential derived from the atomic/molecular electron charge density. Another group Uddin et al [14] apply MRIBED model to calculate the EI single ionization cross sections on a number of targets with atomic number Z = 1–92 in H and Li isoelectronic sequences. The interaction of an electron with cluster provides a valuable probe. In many experiments the clusters are detected due to electron impact ionization in combination with mass spectrometery [15]. Impact ionization cross section are up-to-date there seems to be only measurement of Baba et al [16] for the ionization of C_{60} and C_{70} due to electron impact. Cross section function for C_{60} clusters have been measured by Scheier et al [17] while ionization spectra appearance energies for single and double ionization of C_{60} are recorded by Srivastava et al [18]. In the present study we proposed to modify the Khare et al model to obtaine reliable ionization cross sections over a wide energy range. A detailed investigation will be carried out to apply this model to determine ionization cross sections of bigger atoms and molecules and also for dissociative ionization The impact energy is varied from the ionization threshold I to 3 Mev. To the best our knowledge it will be the first calculation over such a wide energy range.

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Computational Atomic Physics in the e-Science Environment

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Abstract
The perspectives and challenges of computational atomic physics in the new *e-Science* environments are briefly discussed, in particular with reference to code upgrading and the need of a markup language to identify and document atomic and molecular data sets in distributed data repositories.

1. Introduction

This report is based on a talk that was presented at the XVI NCAMP in Mumbai (Jan. 8-11, 07), and is concerned with the perspectives and opportunities that are opening for large-scale projects in computational atomic physics in the new *e-Science* environment. We give an account in Section 2 of the computational projects where we have participated, followed in Sections 3-5 by brief descriptions of the concepts of *e-Science*, grid computing and dataspaces. Some of the problems and challenges that have been encountered in adapting our enterprise to the new cyberinfrastructure are discussed.

2. Large-scale computational atomic physics

Since the mid 80s, we have taken part in long-term, international collaborations to compute massive and accurate atomic data sets for astrophysical applications; namely, the Opacity Project [1] and the Iron Project [2]. These initiatives have involved research groups from Canada, France, Germany, United Kingdom, USA and Venezuela. The computer programs that have been used in these projects include well established atomic structure packages such as SUPERSTRUCTURE [3] and CIV3 [4] and the *R*-MATRIX suite of codes [5] for electron impact excitation of ions. Since most cosmically abundant elements are light ($Z \leq 28$), relativistic effects have been accurately treated as Breit-Pauli corrections. Considerable efforts have also been given to user data accessibility through the implementation and maintenance of databases (TIPTOPbase [6]) and data servers (OPserver [7]) with the kind support of data centers: the CDS [8], HEASARC [9] and the Ohio Supercomputer Center [10].

Although these projects have been productive, both in terms of papers and useful data, they still fall short of current astrophysical data requirements; e.g., a complete atomic database for NLTE modeling, *K*- and *L*-vacancy level energies of spectroscopic accuracy and their decay (radiative and Auger) trees, heavy ions ($Z > 28$) and molecular data in general. In tokamak fusion research, there is need for atomic data for the heavy element tungsten ($Z = 74$). We may conclude that there is an ever present need for massive calculations of atomic and molecular data.

3. What is *e-Science*?

In the words of one of its main promoters, John Taylor (former Director General of Research Councils, UK Office of Science and Technology), *"e-Science is computationally intensive science"*. He has also claimed with much conviction that *"e-Science will change the dynamic of the way science is undertaken"*. In essence, it is computationally intensive science but at a much larger scale, where global distributed collaborations use the Internet as an advanced research environment to mine large volumes of scientific data, to perform terascale simulations and maximize insight through high-performance visualizations. At present, *e-Science* is driven by traditional data-oriented fields such as particle physics (Large Hadron Collider), nuclear fusion (International Thermonuclear Experimental Reactor) and astronomy (Virtual Observatory), but also by newcomers such as the biosciences (genomics, proteomics, pharmacogenetics, bioinformatics), climatology and the social sciences. The unprecedented data deluge that is expected and, by comparison, the shortage of qualified manpower to cope with it, particularly in data processing, communication, storage and curation, are making the integration of research groups from developing countries a main issue.

Since computational atomic physics has always responded to challenging data demands in fields such as astrophysics and fusion plasmas, massive computations and data activities are bound to prosper in the new *e-Science* environment. However, it will require some upgrading of the computational portfolios to the grid and of databases to the new concept of "dataspaces". These topics will be briefly discussed in the following sections.

4. Grid computing

The cyberinfrastructure required for *e-Science* is currently based on the grid computing paradigm which adopts the model of electric power grids; namely, the secure global access, pooling and sharing of distributed heterogeneous computer resources across organizational boundaries. Selection and aggregation of resources at runtime mainly depend on user trustworthiness and quality-of-service requirements since interconnected capabilities will abound; moreover, the grid basic architecture is service-oriented in order to facilitate the formation and management of virtual organizations [11, 12].

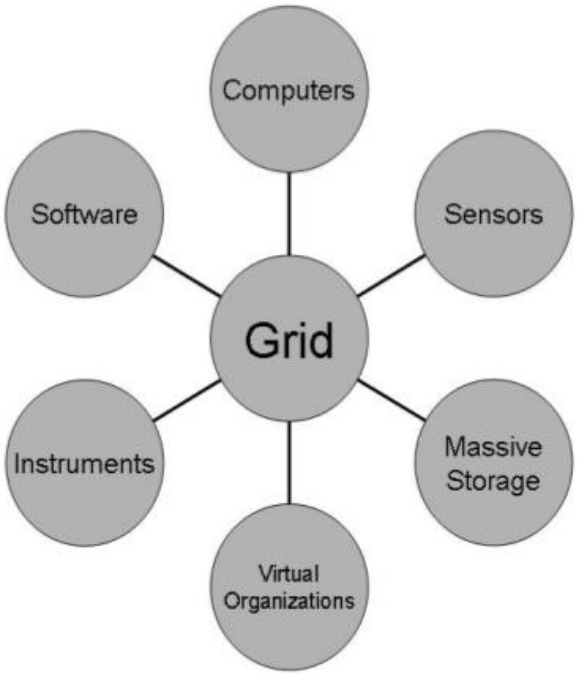

Figure 1: *Scientific grid components*

In Fig. 1 we depict the components of a typical scientific grid. A virtual organization of researchers will have real-time access to large volumes of data being outpoured by sophisticated instrumentation (e.g., an accelerator [13]) or sensor networks [14], but also the possibility of mining large, distributed data archives (e.g., the Virtual Observatory [15]) and using software tools for simulations and modeling on scalable computer platforms (e.g., the European grid EGEE [16]). Grid integration has also been encouraged which may certainly lead to effective solutions for the computing needs and personnel training in developing countries; e.g., the shared infrastructures between Europe and Latin America (EELA [17]) and between Europe and India (EU-Indiagrid [18]), the latter with key applications in high-energy physics, material science, bioinformatics and earth and atmospheric science.

In computational atomic physics, packages such as the *R*-MATRIX [5] are run in stages (see Fig. 2). Each stage reads an input file, writes an output listing and generates sizeable (several GB) intermediate files; the latter are then read by the subsequent stage. Most stages have been already parallelized for cluster platforms, but in order to perform massive calculations in grid environments, it will be necessary to test, revise, upgrade or even change these types of scheme.

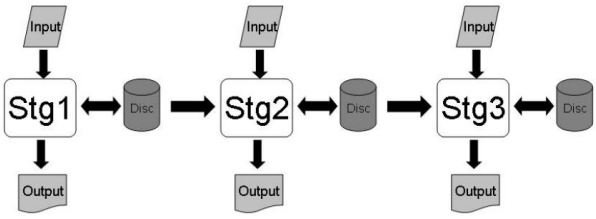

Figure 2: *Scientific applications (e.g.,* R*-MATRIX [5]) are usually run in stages with large intermediate files*

Since most virtual-organizations will interact with the grid through web portals [19, 20], substantial code restructuring must be performed. The familiar monolithic fortran source, say, must now be replaced by a triangular structure distributed between a supercomputer, a web server and a web client (see Fig. 3). The supercomputer may change each time the code is run as well as the web client. Programmers must then be proficient with new resources such as CGI-scripts, HTML and Java, apart from the intricacies of the grid middleware (Globus[21], gLite [22]).

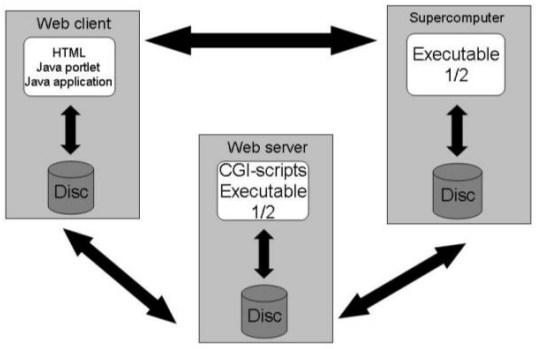

Figure 3: *Triangular structure of scientific applications on the grid*

In interfacing legacy Fortran codes with web portals, we have found that the traditional computing job (compilation – runtime – input reading – data generation – output writing) is no longer practical (see Fig. 4a). It is now more convenient to reorganize it with a database-centric scheme where jobs are handled though a database management system (DBMS, see Fig. 4b).

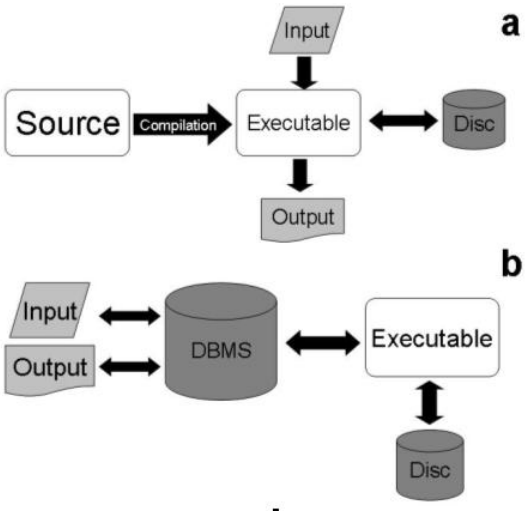

Figure 4: *Traditional computing job. (b) Database-centric job which is found to be more practical in web-interfaced applications.*

5. From databases to "dataspaces"

The Opacity/Iron Projects have always been concerned with aspects related to data storage, accessibility and dissemination, which with the advents of the Internet and the web have reached a high degree of versatility. For instance, in the implementation of an online server of astrophysical opacities, referred to as the OPserver [7], we have considered three user modes (see Fig. 5) which illustrate the different ways in which atomic data are required in user applications. In Mode A, the user downloads the complete database locally for intensive access by a modeling code. In Mode B data are also recurrently fetched by the application but this time from a remote central facility through a network subroutine library. This option is practical for a distributed grid environment where the regular network transfer of the complete database, such as in Mode A, would impact performance. Mode C is aimed at the casual user that queries the remote database and downloads data files through a web page.

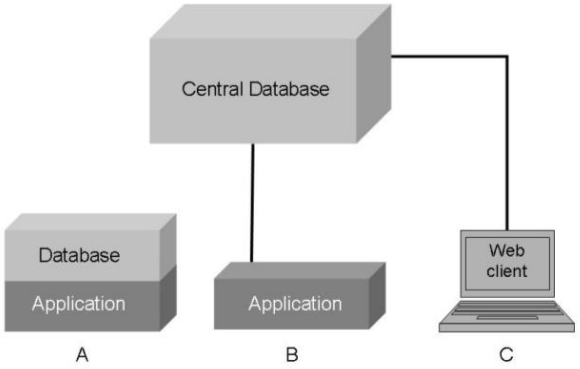

Figure 5: *OPserver user modes. (A) The database is downloaded locally and interfaced with the use application. (B) The user application accesses the remote database. (C) Database is accessed through a web page.*

However, these data access modes do not suffice the envisioned *e-Science* requirements. In future scenarios, most of the data sets will be housed in distributed repositories that do not necessarily comply with a standard data model or the specific structure of a DBMS. Administrative coordination and semantic integration of such data sets can be very low. One must then begin to think in terms of "dataspaces"and Data Space Support Platforms (DSSP) [23] rather than DBMSs. DSSP must then handle different data formats, interfaces and DBMSs, and allow searches and queries even when not having complete control of the data sets; i.e., a query result may only be approximate. An important point is to develop comprehensive metadata that can be readily picked up by the new generation search engines (e.g., Google), and to implement a custom markup language (XML, [24]) for the exchange of atomic and molecular data. An "Atomic and Molecular Data Markup Language"(AMDML) is currently be-

ing developed by an international group led by Yuri Ralchenko (NIST, USA) which will give atomic data sets a flexible yet standardized semi-structure and promote their cataloguing in Google searches.

Acknowledgements
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Royal Society grants for UK-India collaborations May and June 2007 Deadlines

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The Royal Society in the UK has announced its next call for grants to establish (and develop) links between UK and Indian researchers.

1. Fellowships for Indian researchers to be held in the UK

Research fellowships for Indian researchers lasting 6 to 12 months are offered with a **Deadline of May 3**rd. Incoming Fellowships are open to Postdoctoral Researchers based in India (who are Indian Nationals) to undertake high quality research in centres of scientific excellence in the UK. Scientists in the final year of their PhD can submit an application; if successful, the award will only be given subject to the confirmation of their PhD at the time when the award is taken up. The research undertaken must be on a subject within the natural sciences, including: physics, chemistry, mathematics, engineering science, agricultural and medical research, the scientific aspects of archaeology, geography, experimen-

tal psychology and the history of science. UK hosts must hold a permanent or fixed term contract in an eligible organisation which, if it is the latter, continues at least for the duration of the fellowship. Substantial contact between host and candidate prior to the application is essential.

The Royal Society awards are £18,200 per annum (£20,000 in London) - payments are made in quarterly instalments. The award includes £1,000 to enable the candidate to carry out subsidiary scientific visits within the UK and Europe during the course of the fellowship and up to £1,000 claimable by the UK host institution for expenses associated with the candidate's research.

Applications can only be submitted online on the Royal Society's electronic Grant Application and Processing (e-GAP) system https://e-gap.royalsoc.ac.uk/ by the UK (host) Scientist.

2. Royal Society/CSIR India-UK Industrial Research Fellowships Programme.

In addition to the Fellowship scheme discussed above in 2007 the Royal Society has initiated the Royal Society/CSIR India-UK Industrial Research Fellowships programme aims to foster science and technology links between the UK and India, and in particular to enhance knowledge transfer in science and technology between CSIR laboratories in India and UK industry and/or academia. The terms are the same as for the academic fellowship scheme except quoted payments are slightly different, up to one year's subsistence costs at fixed levels of £16,200 per annum, or £18,000 in London, travel and research expenses of £2000. The international travel costs will also refunded on receipt of a claim after the award is made. UK universities will also be awarded a contribution towards FEC overheads.

The CSIR runs a parallel scheme, covering expenses for UK scientists or industrialists to spend time at a CSIR laboratory in India. Enquiries about application for a Fellowship in India at a CSIR laboratory should be directed to CSIR.

3. Short Visits to/from UK

Next deadline is 21 May then 21 August and 21 November.

Shorter visits by Indian Scientists to the UK are supported under the Short visit Scheme. The short visit scheme aims to supports new and on-going international collaborations by providing grants to support an Indian Scientist visiting a UK scientist for between and . The objectives of this scheme are to initiate one to one collaborations, explore opportunities to build lasting networks and gain access to complementary equipment, data, observations and ideas. **Funding is available up to a maximum of 12 weeks and covers only local travel costs and subsistence costs.**

The scheme is for scientists who are working at postdoctoral level. Next deadline is 21 May. Results are normally within 8-10 weeks of the closing date. Visits should be no sooner than 3 months after the closing date.

4. Joint Projects;

Deadline 13 June. Awards will be announced 12 weeks after the closing date

The Royal Society Joint Project programme is designed to enable international collaboration by providing a mobility grant for researchers to cover travel, subsistence and research expenses. The collaboration should be based on a single project including two teams or individuals: one based in the UK and the other based outside the UK. *A relationship between both parties should already be established prior to making an application.* The collaboration should involve bilateral visits between the UK and the country with which the overseas collaborator is based.

Joint Projects are intended for UK and overseas scientists of proven research ability. The Project Leaders must be of at least postdoctoral status or equivalent.UK collaborators should be resident within the UK. The UK applicant must hold a permanent or fixed term contract in an eligible organisation which, if it is the latter, continues at least for the duration of the project. **Project teams must be from academia and not industry**.

Duration of the Joint Project grant and value of awards

The Joint Project scheme runs for two years. The Joint Project grant provides a maximum of £6000 per year. This may be used to claim the costs of travel and subsistence. Within the £6000 cap, the UK Leader may request up to £1000 maximum for research expenses.

Should you require further information look at the Royal Society website http://www.royalsociety.co.uk/ or contact me at n.j.mason@open.ac.uk.

Announcements

Fixed-term position : Compact coherent X-ray source from ultracold atoms

We are looking for a highly motivated and independent researcher to work with us in developing an innovative coherent X-ray source. The source will be based on Inverse Compton scattering of femtosecond laser pulses from ultrabright electron pulses. Cold electrons will be extracted from ultracold plasma formed by photoionisation of ultracold atoms. You must have a PhD in physics, with an experimental background preferably in atom optics, or in optical physics, ultrafast lasers, and/or compact charged-particle accelerators.

For further information, please see http://optics.ph.unimelb.edu.au/jobada4.html

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Workshop on coherent control of optical phenomena - July 9–10, 2007

Indian Institute of Technology, Kanpur, India

The workshop will focus on various aspects of coherent light-matter interactions that result in the control of properties of both the material and the fields. Recent progress in this area will be discussed and the workshop will also aim at providing basic understanding of a variety of counterintuitive control phenomena.

Topics

Coherent control in Nonlinear optics
Coherent control and generation of Atomic coherence
Coherent control of dynamics in atoms and molecules
Electromagnetically induced transparency
Coherent control in Quantum Information science
Coherent control in Bose-Einstein condensates
Coherent Control of decay processes and decoherence
Coherent control and generation of Non-classical light
Coherent control of wavepacket dynamics

Leading experts in this field will participate in the workshop which will also have sufficient pedagogic content aimed at graduate students and researchers who wish to venture into this area of research.

For further information, participation and registration, kindly contact

Dr. Harshawardhan Wanare (*Organizing Secretary*)
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hwanare@iitk.ac.in

Honours

- Dr. Bhas Bapat, Physical Research Laboratory, Ahmedabad *(also, Treasurer, ISAMP)* has been elected as an Assoiciate Member of The Gujarat Acadamy of Sciences.

- Professor Tapan Ganguly, Head, Department of Spectroscopy, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, has been elected as a fellow of the West Bengal Academy of Sciences and Technology (FAScT).

- The research paper titled *"Measurement of the van der Waals force using reflections of cold atoms from magnetic thin-film atom mirrors"* by Prof. C.S. Unnikrishnan's group at TIFR, Mum-

bai has been selected as a highlight from those articles published by the Europhysics Letters (EPL) journal in 2006. A special collection of 'highlight'articles has been created at http://herald.iop.org/epl/m4/gzw/179656/link/610.

- Dr. Arun K. Pati's work establishing that quantum information cannot be completely hidden in correlations *(abstract no. 6 cited in this issue of newsletter)* has been acclaimed in the Indian media. A detailed news had recently appeared in Indian Express (http://www.indianexpress.com/story/25433.html)

Obituary

Prof. M.B. Kurup Department of Nuclear and Atomic Physics, TIFR, Mumbai passed away on Sunday, 8th April, 2007. He was the In-charge of the Pelletron accelerator facility and the superconducting LINAC booster. He had played a leading role in the development of the LINAC booster at TIFR. His research interest was spread over many areas in physics, such as accelerator based atomic physics, ion-solid interactions, beam-foil spectroscopy, crystal channelling and blocking measurements for nuclear lifetime studies and ion-beam modifications of materials such as metals, oxides and semiconductors. Prof Kurup has served as the Dean of Natural Science Faculty of TIFR until very recently. He was highly respected across the entire community, even outside the scientific community. He has served as a Member of Council of a few DAE institutes, and also has served in many committees constituted by DAE. He was a member of ISAMP and has always been very supportive of the community.