Schedule

Time table	Wednesday, July 27	Thursday, July 28		Friday, July 29		Saturday, July 30	
08:20 - 08:30 hs		Opening Remarks		-		-	
08:30 - 09:30 hs		S. J. Buckman		M. Charlton		F. A. Gianturco	
09:30 - 10:00 hs		Coffee Break		Coffee Break		Coffee Break	
10:00 - 10:30 hs		P. Kolorenc	C. Y. Ho	L. G. Ferreira	G. P. Karwasz	C. Winstead	J. A. Young
10:30 - 11:00 hs		A. Wolf	G. F. Gribakin	C. S. Trevisan	W. E. Kaupilla	R. Johnsen	R. J. Bunker
11:00 - 11:30 hs		A. F. Borghesani	E. A. G. Armour	T. A. Field	S. Jonsell	Panel Session on Opportunities and Challenges	M. Bromley
11:30 - 12:00 hs		N. J. Mason	A. S. Ghosh	C. Makochekanwa	D. B. Cassidy		Panel Session on Opportunities and Challenges
12:00 - 12:30 hs		M. Radmilovic	R. O. Barrachina	P. Scheier	F. Arretche		
12:30 - 14:00 hs		Special Lunch		Lunch		Closing Remarks and Lunch	
14:00 - 14:30 hs		K. Morgenstern	S. Armitage	M. A. Khakoo	Y. Nagashima	Additional information 1) Please, wear your badge at all times in order to help interaction between the two communities. 2) You have registered in only one conference, but free transit is allowed between sessions. 3) All meals are included in your registration fee and you will receive tickets related to them. Regular meals will be at a nearby restaurant and includes soft drink and dessert. 4) Buses to (from) Comfort Suites and Sleep Inn hotels will be provided at specific times. CPV is at walking distance of the conference site.	
14:30 - 15:00 hs		Y. Sakai	C. Arcidiacono	M. Takahashi	L. V. Jorgensen		
15:00 - 15:30 hs	Registration and Welcome Reception	L. A. Viehland	H. R. J. Walters	J. Tennyson	N. Oshima		
15:30 - 16:00 hs		J. de Urquijo	J. P. Marler	T. Sommerfeld	H. Saito		
16:00 - 16:30 hs		Coffee Break		Coffee Break			
16:30 - 17:30 hs		G. Gabrielse		H. Hotop			
17:30 - 19:00 hs		Poster Session		Poster Session			
19:00 - 20:00 hs		Dinner and IOC Meeting		Conference Dinner			
20:00 - 21:00 hs							
20:30 - 22:00 hs							

International Workshop on Low Energy Positron and Positronium Physics

27-30 July 2005
Campinas, SP, Brazil

Editors:
Sergio d'A. Sanchez
Romarly F. da Costa
Marco A. P. Lima

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Preface

It is with great honor that the Local Organizing Committee welcomes the participants of the XIII International Workshop on Low-Energy Positron and Positronium Physics in Campinas, Brazil - a satellite meeting of the XXIV International Conference on Photonic, Electronic and Atomic Collisions, in Rosario, Argentina.

This is the first time the Workshop is held in South America and we sincerely hope this will stimulate the development of the field in the whole Continent, as indicated by the record number of contributed papers from South American countries.

This meeting, with its 26-year tradition, is also held for the first time in conjunction with the International Symposium on Electron-Molecule Collisions and Swarms. There is an overlap between these two fields, with some of the researchers working on both areas, and this shall provide a profitable interchange for both communities.

Finally, we would like to acknowledge the help from the International Advisory Committee, the support provided by the Brazilian Physical Society in many ways, and those who willingly helped making this Workshop feasible.

Marco A. P. Lima, Chair
Local Organizing Committee
of the XIII International Workshop
on Low-Energy Positron and Positronium Physics

July, 2005

Conference General Information

1. Conference Site

"The University of Campinas was established in 1966, as a public university funded by the State of São Paulo. Its mission is to provide education and training, qualifying our students to play a key role in the process of social development. Unicamp seeks to contribute in the solution of social problems, through education, research and also through services to the community.

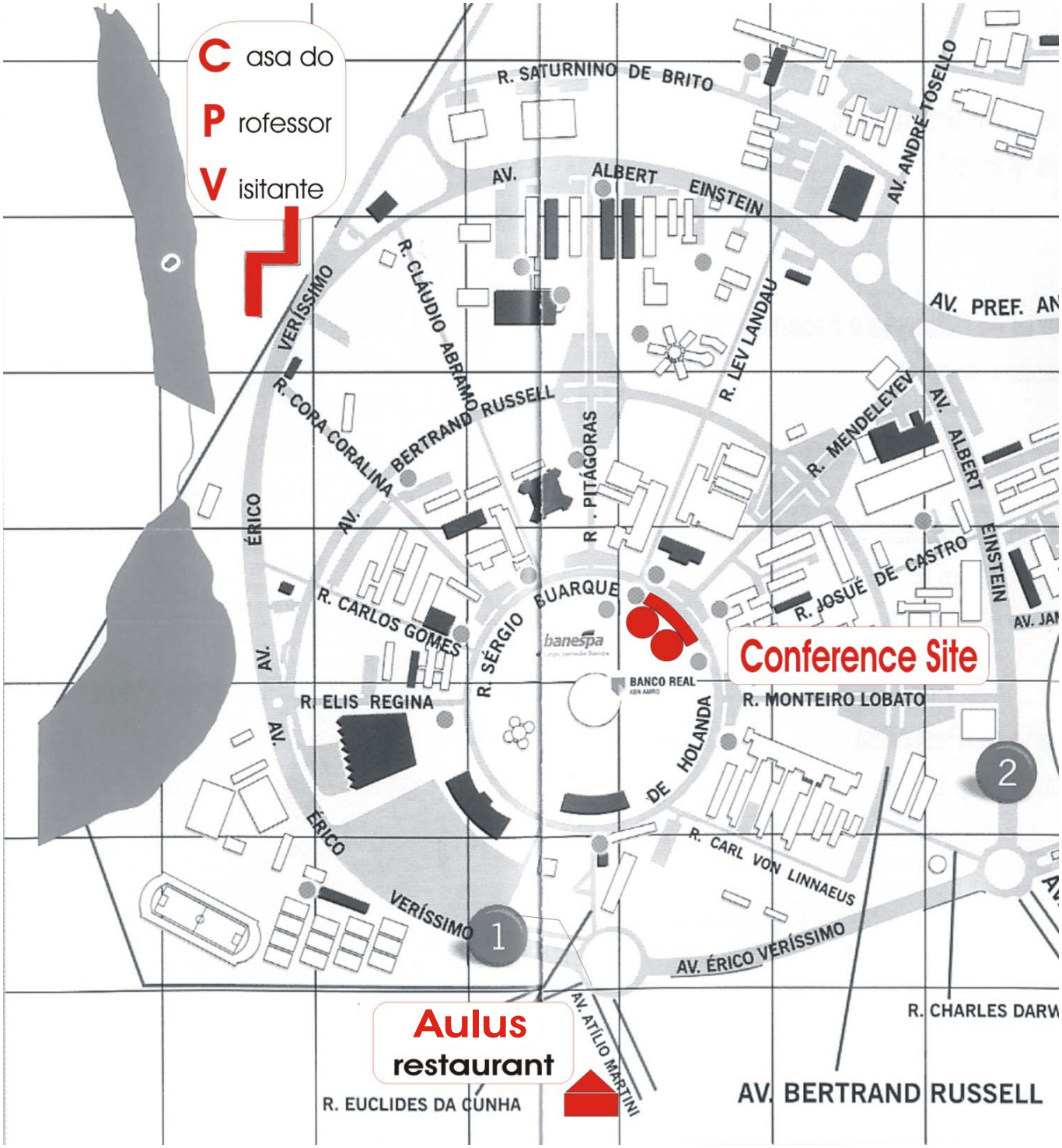
A healthy balance between research and teaching, pure and applied science has made Unicamp one of the most distinguished Brazilian academic Institutions. Unicamp receives undergraduate and graduate students from all over Brazil and also from abroad.

In Europe and even in the American Continent, the history of the oldest universities spans over centuries, while in Brazil it can still be counted in decades. Furthermore, if the history of the Brazilian university is recent, that of the State University of Campinas (Unicamp) is even more. Unicamp had its campus officially opened on October 5th 1966. Few years later it was already recognized as one of the leading Brazilian and Latin American institutions of higher education, conducting advanced research and tackling important social issues. Today, Unicamp can be considered as a fully consolidated university.

Unicamp combines its youth with a strong experience in producing new knowledge in virtually all areas. In effect, today, the University concentrates 15% of the total scientific production in this country and approximately 10% of the graduate courses. The result is its capability to maintain areas of scientific and technological compatibility with the main research centers in the world, through numerous international cooperation agreements. Unicamp is an autonomous autarchy of the São Paulo State. Financial resources are obtained mainly from the state government. Funding is also provided by national and international research funding agencies. Students do not pay tuition fee, since the University is financed by state funds", (from UNICAMP webpage)

The meeting will take place at Ciclo Básico I, a building specially designed to accommodate basic-level undergraduate classes, taken by most of Unicamp students. The classrooms are connected to high speed internet and have the necessary infrastructure for the Positron-05 meeting. A Campus map indicating the most important sites of the Workshop is shown below.

Map of Campus



2. Meals

The registration fee includes all the meals served during the Conference, and tickets will be provided for all participants. We request that you always bring the tickets to the restaurants, and also that you wear your badge at all time.

The Welcome Reception will be held at the Ciclo Básico I from 18:00 – 21:00 h July, 27.

A Special Lunch will be served on Thursday at Coxilha Grill, a famous “all you can eat” barbecue restaurant in Campinas. It offers a rich salad bar and about 26 different kinds of meat. The tickets will also include beer, mineral water, soft drinks, juices and dessert (ice cream).

Regular meals will be served at Aulus restaurant, located just outside the Campus (see the map). The tickets include the main dish, a soft drink and a dessert. Aulus is a self-service restaurant, so you are invited to help yourself. They have a large selection of salads, cold dishes, hot dishes, typical Brazilian juices and desserts.

The Conference Dinner will take place at Alphaville Club with typical Brazilian dishes (mainly fish and seafood, but there will be an alternative menu for vegetarians), provided by Idalvo’s, another very popular restaurant in Campinas.

The Farewell Lunch will be held at CPV. Nothing could be better to close the Symposium than the most famous Brazilian dish: feijoada, prepared with black beans, rice and pork.

Tickets will be provided to accompanying persons for the Welcome Reception and Conference dinner, and will be sold at the Conference desk for the other meals.

3. Ground Transportation

If you are staying at Comfort Suites or Sleep Inn, the Conference will provide ground transportation from/to these hotels to the Conference Site at scheduled times. On Wednesday, buses will take you to your hotel after the Welcome Reception at 21:00 h. On Thursday, Friday and Saturday buses will depart from the hotels at 08:00 h, and on Thursday they will leave Unicamp at 21:00 h. Those staying at Casa do professor Visitante (CPV), may walk to the Conference site (about five minutes).

Ground transportation will also be arranged for all participants for the Special Lunch and the Conference Dinner.

In the last day of the Conference, please leave your luggage at the hotel after checking-out. A bus to Guarulhos International airport will leave CPV after the Farewell Lunch at 15:30.

4. Poster Prize

We have the pleasure to announce that there will be a selection for the best poster of the meeting. The prize, in the amount of US$ 175,00, was donated by Clifford M. Surko, Gleb F. Gribakin, and Helge Knudsen. The donors have requested that their posters as well as those of their co-workers should not be considered for election.

You will receive a voting ticket at the registration desk upon arrival. We will also have, at the same location, a place to cast your vote after making your decision (votes must be deposited by July 30th, Saturday, 10:00hs).

The result will be announced at the closing remarks just after the last session of the Conference.

5. Internet

Computers will be available at the Conference desk for participants to access the Internet.

6. Important Information on Campinas and Brazil

Electric power - In Campinas, the voltage is 110 V - 60 cycles, unless indicated otherwise, though most of the hotels have sockets for both 110 and 220 V.

Business Hours - Most stores open from 09:00 h to 18:00 pm on weekdays, and from 09:00 h to 13:00 h on Saturdays. Some malls are open up to 22:00 h on weekdays and on Sundays afternoon. Bank branches open from 10:00 h to 16:00 h, only on weekdays.

Car rental - As previously stated, ground transportation will be provided by the conference, but car rentals, with or without drivers, are available at all major international airports.

Taxis - There are a lot of taxis in Campinas and they may be called at the hotel desk. Most of the taxi drivers, however, do not speak any other language than Portuguese.

Tipping - A 10% tip is already included in the bill of most restaurants. If not included, the general rule is to give a 10% tip. Taxi drivers do not expect tips.

Scientific Program of the International Workshop on Low-Energy Positron and Positronium Physics

All sessions are in Ciclo Básico I – room CB02, except the plenary lectures and the opening and closing remarks, which are on room CB01

Wednesday, July 27

15:00 – 21:00

Registration

18:00 – 21:00

Welcome Reception

Thursday, July 28

08:20 – 08:30

Opening Remarks

08:30 – 09:30
Plenary Lecture A – Chair: Franco A. Gianturco

Stephen J. Buckman, The Australian National University, Australia
Benchmark studies of electron (positron)–molecule (atom) scattering

09:30 – 10:00
Coffee Break

Session A – Chair: Walter E. Kaupilla

10:00 – 10:30

Chi Yu Hu, Department of Physics, CSULB, USA
Positron annihilation

10:30 – 11:00

Gleb F. Gribakin, Queen's University, Belfast, UK
Many-body theory of positron-atom interactions

11:00 – 11:30

Edward A. G. Armour, Nottingham University, UK
Matter-antimatter interactions involving antihydrogen

11:30 – 12:00

Arnab S. Ghosh, Indian Association for the Cultivation of Science, India
Electron-positronium scattering and Feshbach resonances

12:00 – 12:30

Raúl O. Barrachina, Centro Atómico Bariloche and Instituto Balseiro, Argentina
Theory of ionization processes in positron-atom collisions

12:30 – 14:00
Special Lunch

Session B – Chair: Gleb F. Gribakin

14:00 – 14:30

Simon Armitage, University College London, UK
Collisions involving positronium

14:30 – 15:00

Cristiana Arcidiacono, University College London, UK
Differential studies of positron impact ionization

15:00 – 15:30

H. R. J. Walters, Queen's University, Belfast, UK
Positronium fragmentation

15:30 – 16:00

Joan P. Marler, University of California, San Diego, USA
New results in positron scattering from noble gas atoms and diatomic molecules

16:00 – 16:30
Coffee Break

16:30 – 17:30
Plenary Lecture B – Chair: Edward A. G. Armour

Gerald Gabrielse, Harvard University, USA
Positron quantum cyclotron and antihydrogen

17:30 – 19:00
Poster Session

19:00 – 21:00
Dinner and IOC Meeting

Friday, July 29

08:30 – 09:30
Plenary Lecture C – Chair: Cláudio L. Cesar

Michael Charlton, University of Wales Swansea, UK
Progress with cold antihydrogen

09:30 – 10:00
Coffee Break

Session C – Chair: Gaetana Laricchia

10:00 – 10:30

Grzegorz P. Karwasz, Università di Trento, Italy
Total cross section for positron scattering on noble atoms and cyclic hydrocarbons

10:30 – 11:00

Walter E. Kauppila, Wayne State University, USA
Investigations of positronium formation and destruction using PsARS

11:00 – 11:30

Svante Jonsell, Umeå University, Sweden
Low-temperature antihydrogen-atom scattering

11:30 – 12:00

David B. Cassidy, University of California, Riverside, USA
Creation and observation of di-positronium molecules

12:00 – 12:30

Felipe Arretche, Universidade Estadual de Campinas, Brazil
Electronic excitation of H_2 by positron impact

12:30 – 14:00
Lunch

Session D – Chair: Clifford M. Surko

14:00 – 14:30

Yasuyuki Nagashima, Tokyo University of Science, Japan
Inner shell ionization by positron impact

14:30 – 15:00

Lars V. Jorgensen, University of Wales Swansea, UK and CERN, Switzerland
Positron physics in antihydrogen production - a look to the future

15:00 – 15:30

Nagayasu Oshima, RIKEN and AIST, Japan
Positron accumulation in ultra high vacuum with an electron plasma

15:30 – 16:00

Haruo Saito, University of Tokyo, Japan
Positron and positronium interactions in solids

16:00 – 16:30
Coffee Break

16:30 – 17:30
Plenary Lecture B – Chair: Ann E. Orel

Hartmut Hotop, Universität Kaiserslautern, Germany
High resolution studies of dissociative electron attachment to molecules

17:30 – 19:00
Poster Session

19:00 – 22:00
Conference Dinner

Saturday, 30

08:30 – 09:30
Plenary Lecture E – Chair: Hiroshi Tanaka

Franco A. Gianturco, The University of Rome “La Sapienza”, Italy
Modelling dynamical processes in molecular gases induced by low-energy positrons

09:30 – 10:00
Coffee Break

Session E – Chair: Gerald Gabrielse

10:00 – 10:30

Jason A. Young, University of California, San Diego, USA
New results on positron-molecule annihilation, vibrational Feshbach resonances and bound states

10:30 – 11:00

Robert J. Buenker, Bergische Universitaet Wuppertal, Germany
Positron binding energies for alkali hydrides

11:00 – 11:30

Michael W. J. Bromley, Charles Darwin University, Australia and Kansas State University, USA
Calculations of positron interactions with one- and two-electron atoms

11:30 – 12:30

Panel Session on Opportunities and Challenges – Chair: Clifford M. Surko

12:30

Closing Remarks

12:30 – 14:00
Lunch

List of Invited Papers

List of Contributed Papers

LIST OF INVITED PAPERS

Using the scattering solutions of the modified Faddeev equation, we find that it is possible to effectively separate out the singular part of the effective charge integral Z_{eff} and obtain stable converged values for Z_{eff} in all incoming channels. We carried out numerous calculations in the Ore gap where there are two open channels. For the e^++H($1S$) incoming channel, Z^1_{eff} has converged within 2% for a wide range of cut-off radii as well as various combinations of the splitting parameters in the modified Faddeev equation as long as the respective K-matrices are relatively converged (within 10% accuracy). However, Z^2_{eff} corresponding to the incoming channel p+PS($1S$) are much more critical of our numerical accuracy. Only those wave functions having K-matrix accurate within 1% produce stable Z values. We will discuss the source of this problem in detail. We find that all the Z_{eff} behave smoothly within the Ore gap except near resonances. The characteristics sharp raise in Z just before a Feshbach resonance and a dip very near the resonance is observed in all cases calculated.

MANY-BODY THEORY OF POSITRON-ATOM INTERACTIONS

G. F. Gribakin*

Department of Applied Mathematics and Theoretical Physics, Queen's University Belfast, UK

Many-body theory is an attractive alternative to solving the Schrödinger equation for a system of interacting particles. It allows one to visualise the processes which take place and to consider the role of different mechanisms, without compromising the quantum-mechanical description of the system. The language of Feynman diagrams serves as a universal book-keeping tool for the contributions to the amplitudes of various processes, and is amenable to one's use of physical intuition.

Within the many-body theory formalism, the scattering of a positron by an atom is described by the Dyson equation,

$$H_0\psi(\mathbf{r}) + \int \Sigma_\varepsilon(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}' = \varepsilon\psi(\mathbf{r}), \qquad (1)$$

where H_0 is Hamiltonian of the positron in the static field of the target (described at the Hartree-Fock level), $\psi(\mathbf{r})$ is the quasiparticle wavefunction of the positron, and $\Sigma_\varepsilon(\mathbf{r},\mathbf{r}')$ is the positron-target *correlation potential*, which depends on the positron energy ε. Although equation (1) has the form of a single-particle Schrödinger equation, the nonlocal potential Σ_ε accounts for all the many-body interactions. It can describe elastic and inelastic scattering. The positron wavefunction $\psi(\mathbf{r})$ can be used to determine the annihilation rate and gamma spectrum. (This also requires inclusion of nonlocal corrections to the *annihilation vertex*, similar to Σ_ε.)

Applied to the positron-atom interaction problem, many-body theory has provided a number of important insights into the physics of this interaction.

- Virtual positronium formation gives a large contribution to the positron-atom correlation potential [1, 2, 3].
- Strong positron-atom attraction gives rise to low-lying positron virtual states (e.g., in Ar, Kr and Xe [2, 5]), and positron binding to neutral atoms [4].
- Positron-atom virtual states are responsible for large values and strong energy dependence of positron annihilation rates on noble gases.
- Short-range electron-positron correlation effects enhance the annihilation rate several times, and have a weak dependence on positron energy [2, 5].
- The formalism can be extended to positron energies above the Ps formation threshold, to describe Ps formation and direct ionization [6].
- Virtual positronium formation and the short-range correlation effects can be accurately included by calculating the electron-positron vertex function [7].

Combined with modern age computer facilities, the many-body theory allows one to develop an accurate quantitative theory of positron-atom scattering, binding and annihilation [7].

* This work was started in collaboration with V. A. Dzuba, V. V. Flambaum and W. A. King. John Ludlow and Louise Dunlop played a key role in the recent developments.

References

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MATTER-ANTIMATTER INTERACTIONS INVOLVING ANTIHYDROGEN

E A G Armour*, S Jonsell#, Y Liu* and A C Todd*

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\# Department of Physics, Umeå University, SE-90187 Umeå, Sweden

The ATHENA and ATRAP projects are continuing their work on antihydrogen at CERN after their successful preparation of antihydrogen in 2002. See, for example, [1,2]. This has opened up the prospect of a whole new area of investigation in atomic and molecular physics, in addition to tests of the CPT invariance of relativistic quantum field theory and Einstein's principle of equivalence.

The simplest interaction to consider is between atomic hydrogen and antihydrogen. We have already carried out calculations of cross sections for very low-energy hydrogen antihydrogen ($H\bar{H}$) scattering [3,4].

There is currently considerable interest in the interaction of antihydrogen with the next simplest atom, helium, both as a possible means of cooling $\bar{H}$ and as a way of determining the $\bar{H}$ loss rate due to the presence of He as an impurity. We are currently carrying out calculations of very low-energy cross sections for $He\bar{H}$ scattering. We have calculated wave functions and energies for $He\bar{H}$ in the Born–Oppenheimer approximation using basis sets that contain Hylleraas-type functions that correlate the interaction of the positron in $\bar{H}$ with the electrons in He [5].

These calculations give accurate results for the energy but not as accurate as the values obtained by Strasburger and Chojnacki using a basis set made up of explicitly correlated Gaussian functions [6]. Work is currently being carried out on the inclusion of Hylleraas-type functions that correlate the interaction between the electrons. This will bring about an improvement in the accuracy of the energy.

As Strasburger and Chojnacki's energy values are more accurate, we used them to obtain the potential that we required to calculate elastic scattering cross sections. However, our wave functions made it possible to carry out calculations for rearrangement processes. Cross section values for the antiprotonic He + Ps channel will be presented at the conference. These have been calculated using the distorted wave T-matrix approach used by Jonsell et al. in their calculations on $H\bar{H}$ [4]. A progress report will be given on calculations on the $He\bar{p} + e^+$ channel.

Our $He\bar{H}$ calculation will form the starting point for a wide range of applications. The T-matrix approach can be extended to make possible calculations on $He\bar{H}$ scattering using the Kohn variational method, as in the case of $H\bar{H}$ [3]. In addition, our $He\bar{H}$ calculation can be adapted and extended to make it possible to carry out a Kohn calculation of e^+H_2 scattering with inclusion of the Ps formation channel which was not possible in earlier calculations [7].

Together with R-matrix calculations [8], these calculations will be used to make a detailed study of the very high positron annihilation rates that have been observed in positron scattering by some molecules [9,10]. This is supported by EPSRC (UK). One of the smallest target molecules for which the very high annihilation rates have been observed is acetylene, HCCH. A key question is how to represent accurately the short range interaction between the positron and the target electrons in such molecules, for which it is not possible to use Hylleraas-type basis functions.

One possibility is to use Gaussian basis functions. As an indication of what might be expected from such an approach, we will conclude with a comparison between δ-function expectation values for positron-electron coincidence for $He\bar{H}$ calculated using our wave functions containing Hylleraas-type functions and those obtained by Strasburger [11] using explicitly correlated Gaussian functions.

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ELECTRON-POSITRONIUM SCATTERING AND FESHBACH RESONANCES

A S Ghosh

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This progress report details the scattering of electrons by positronium (Ps) atoms and Feshbach resonances up to n=4 threshold due to doubly excited auto detaching states of positronium negative ion (Ps^-) carried out by our group [1,5].

It is of interest to study the spectra of Ps^- and compare it with that of H^-. Present dissertation provides the details of close coupling approximation (CCA) model employed by us. This article also discusses the other elaborate methods already employed to investigate the system [2-4]. Comparisons amongst the predictions by different methods constitute a section in this article.

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Theory of ionization processes in positron-atom collisions

R. O. Barrachina

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We review past and recent theoretical developments in the description of ionization processes in positron-atom collisions. Starting from an analysis that incorporates all the interactions in the final state on an equal footing and keeps an exact account of the few-body kinematics, we perform a critical comparison of different approximations, and how they affect the evaluation of the ionization cross section. Finally, we describe the appearance of fingerprints of capture to the continuum, saddle-point and other kinematical mechanisms.

Abstract for invited talk

Collisions Involving Positronium

S. Armitage, J. Beale, D. E. Leslie and G. Laricchia
Department of Physics & Astronomy, University College London,
Gower Street, London, WC1E 6BT

Recent developments in the production and scattering of the Positronium beam at UCL will be reviewed. The Positronium beam is formed through the charge-exchange reaction of a positron beam within a suitable gas target, utilizing the forward peaked nature of the differential Positronium formation cross-section. Results for the production efficiency of converting a positron into a Positronium beam will be compared for a number of atomic and molecular targets [1-3].

Total cross-sections for Positronium scattering have been measured for a number of simple atoms and molecules [1,4], as well as the fragmentation cross-section of Positronium collision with He atoms [5]. The longitudinal energy distributions of the residual positrons from Positronium fragmentation have also been determined and found to be strongly peaked at half of the residual energy, indicating the occurrence of electron-loss-to-the-continuum. Corresponding investigations of the ejected electrons are underway. Comparisons will be made with theories where available.

With knowledge of both the positron and Positronium total scattering cross-sections and the measurement of the Positronium detection efficiency, absolute differential Positronium formation cross-sections have also been extracted from the Positronium beam production efficiency measurements [6]. Comparisons with theory are made where applicable.

We are grateful to the Engineering and Physical Sciences Research Council for supporting this work under grant no. No. GR/S16041/01.

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In Preparation

Abstract for invited talk

Differential Studies of Positron Impact Ionization

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Differential studies are an important probe of collision dynamics. In a previous study, the occurrence of the electron-capture-to-the-continuum (ECC) for 50eV positron impact ionization on H_2 was investigated [1,2,3]. The possible origins of an observed energy shift between the experimental data and a theoretical distribution have now been investigated. In this study, two targets have been considered at the same final state energy. Molecular deuterium has been used to establish whether at this energy ionization is significantly accompanied by dissociation of the remnant ion. A helium target has also been employed to eliminate possible contributions from molecular excitations. Both electron spectra for D_2 and He have been found to be shifted as for the molecular hydrogen by ~ 1.6eV. In order to understand the energy discrepancy, the scattered positron projectiles have also been energy analysed. The results clearly reveal unexpected asymmetries in the sharing of the residual kinetic energy between ejected electron and scattered positron. Results will be presented at the conference.

This work is supported by the Engineering and Physical Science Research Council UK (grant No. GR/S16041/01), The Royal Society (ref. 60003.P606) and the Hungarian Scientific Research Found (OTKA No. T025325).

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POSITRONIUM FRAGMENTATION

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With increasing impact energy the main outcome of positronium - atom collisions is fragmentation of the positronium (Ps). In a paper published in 2001 Ludlow and Walters [1] put forward some ideas on coincidence studies of Ps fragmentation. In its most rigorous form the kinematics of such a study would be fully determined, ie, one would measure the momentum of the incoming Ps, the momenta of the outgoing electron and positron, and one would have information on the initial and final states of the atomic target. The result of such an experiment would be a triple differential cross section (TDCS). In analogy with (e, $2e$), Ludlow and Walters termed this a (Ps, e^+e^-) measurement. Despite enormous advances in the experimental study of Ps - atom collisions, it will be some time before it is possible to measure a TDCS. However, the first measurement of a single differential cross section has recently been made [2,3], in this case the cross section differential with respect to the longitudinal energy of the ejected positron. These measurements have been made on a He target and at relatively low impact energies ($\leq$33eV). At impact energies below 27eV excitation/ionization of the He is not possible and between 27 and 33eV it should be unimportant.

In this talk I shall look at the theoretical description of Ps fragmentation and what can be learnt from observing the spectra of ejected positrons and electrons. The theoretical description requires account to be taken not only of collisions in which the target atom remains in its initial state but also of situations in which it is excited or ionized. If we observe the ejected electrons rather than the positrons, then we need also to consider electrons that come out of the target atom.

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NEW RESULTS IN POSITRON SCATTERING FROM NOBLE GAS ATOMS AND DIATOMIC MOLECULES

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In this talk, I discuss new data on the formation of Ps atoms by positron impact [1]. Ps formation represents a very significant theoretical challenge. From an experimental point of view, while there have been a number of experimental studies of Ps formation in noble gases, there is significant disagreement as to the magnitude and shape of the cross sections. Additionally, positron annihilation, which frequently occurs via this intermediary Ps state, is frequently exploited in applications of positrons to material science and biophysics.

The experiment described here uses a trap-based positron beam [2] with an energy spread ~ 25 meV (FWHM). It is tunable from ~ 50 meV upwards. The measurements are done in a strong magnetic field (i.e. 0.1 T). Regions of variable magnetic field strength are used to distinguish elastic and inelastic scattering events.

Results will be presented for the absolute direct and total ionization and Ps formation cross sections in Ne, Ar, Kr, Xe, at energies from threshold up to 90 eV. The experimental data for Ps formation will be compared with the most recent measurements of these cross sections obtained using a significantly different technique [3]. There is excellent agreement between the total ionization cross sections. However in the direct ionization and positronium formation there are some significant disagreements (e.g. the previous report of a second peak in the Ps formation cross section in Ar), and they will be discussed.

In addition to the direct measurements of Ps formation, another analysis will be described that provides an independent measurement of the Ps formation cross sections. The results of this analysis and the direct measurements presented here are in good agreement for Ar, Kr and Xe [1]. These results will be compared with previous experimental measurements and with previous and new theoretical predictions. New theoretical predictions for the direct ionization cross sections are in reasonably good agreement with the data. The Ps formation predictions are less able to match the experimental cross sections.

Results for the direct and total ionization of the diatomic molecules, N_2, CO and O_2 will also be presented and compared to other available measurements and theoretical predictions. There is generally good agreement between the present and previous experimental measurements for these targets, thus providing an important benchmark for theory.

Updated and new results for the electronic excitation of N_2 and CO by positron impact will be presented. These isoelectronic diatomic molecules were chosen because N_2 has been shown to be such an effective buffer gas for trapping positrons. Comparison of the new results for Ps formation (the major loss process in buffer gas traps) and the electronic excitation cross sections sheds light on these competing interactions inside a buffer gas trap.

It has been experimentally noted that the addition of CF_4 gas in the third stage of the trap leads to a faster cooling rate. This effect has been investigated by measuring the vibrational excitation cross section of CF_4 as a function of incoming positron energy, and will be presented.

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Positron Quantum Cyclotron and Antihydrogen

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Current measurements illustrate the usefulness of low energy studies of particle properties and fundamental symmetries. A one electron quantum cyclotron -- a single trapped electron cooled to such a low temperature that the quantum structure of its cyclotron motion is clearly resolved -- is used to make a greatly improved measurement of the electron magnetic moment. This measurement, with QED theory, establishes a much more accurate new value for the fine structure constant -- the fundamental measure of the strength of the electromagnetic interaction. A positron quantum cyclotron will produce the most stringent test of CPT invariance with a lepton system. Precise laser spectroscopy or antihydrogen would greatly improve the accuracy at which CPT can be tested with leptons and baryons. Great progress in measuring the velocity and internal orbit properties of antihydrogen atoms brings closer the goal of comparing antihydrogen and hydrogen atoms, using highly accurate laser spectroscopy to provide what likely will be the most strenuous test of CPT invariance with baryons and leptons. A new, laser-controlled method for producing slow antihydrogen is the second of two methods now available to make slow antithydrogen.

Progress with Cold Antihydrogen

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Since 2002, when cold antihydrogen was first produced in the laboratory, there has been an explosion of activity in this field, both experimental and theoretical. Two experiments at CERN, ATHENA [1] and ATRAP [2], both utilising a nested Penning trap technique [3], have driven these advances. Insights have been gained into antihydrogen formation mechanisms and binding energies, the (positron) temperature dependence of antihydrogen formation and the velocity and spatial distributions pertaining to the emitted antihydrogen. We will review this material. Though much remains to be done, current knowledge is pointing the way towards precision spectroscopy with trapped antihydrogen. We attempt an anticipation of these developments and recall the physics motivations for undertaking these challenges.

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Total cross section for positron scattering on noble atoms and cyclic hydrocarbons

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Recently, total cross sections (TCS) for positron scattering on atoms (He, Ar) and molecules (N_2, C_6H_6, $C_6H_5NH_2$, C_6H_{12}) in 0.5-20 eV energy range have been measured at Trento University [1].
The relatively high (from 20 e^+/s to 200 e^+/s) counting rate and a good beam stability allowed to obtain low (below 4%) statistical uncertainty in those measurements; small apertures in the scattering cell (1 mm in diameter) with a rather low (1 mT) transport magnetic field used make the forward scattering error small (less than 10%) even at the lowest energies.
The following consideration obtained from those data will be discussed:

1) TCS in the zero energy limit rise for all studied targets
2) TCS for benzene from Trento are in a good agreement with the recent theory [2]
3) discrepancy on point 1) with the most recent data of Kimura and collaborators [3] come, probably, from their much higher forward scattering uncertainty (6 mm in diameter aare the scattering cell apertures)
4) for Ar and N_2 a constant TCS is observed up to the positronium formation threshold,
5) the rise of TCS at energies above this threshold in Ar can be attributed to the Ps-formation process [4].
6) possible resonances in TCS for positron scattering on atoms and molecules will be discussed.

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Investigations of Positronium Formation and Destruction using PsARS*

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The development of positronium annihilation ratio spectroscopy (PsARS) has been found to be particularly useful for investigations of positronium formation and destruction [1]. This new method of spectroscopy relies on measuring the relative ratio of γ-rays resulting from the annihilation of ortho-Ps to those from the annihilation of para-Ps. Two NaI scintillators with attached phototubes on opposite sides of a positron beam transmission scattering cell are used to detect in coincidence the two 511 keV γ-rays from para-Ps decay and to also detect in coincidence 2 of the 3 γ-rays (in the energy window 300 to 460 keV and completely excluding the 511 keV peak) from ortho-Ps decay.

It has been found [1] that within 2 eV of the initial Ps formation threshold for many target gases that the ratio ($R_{3\gamma/2\gamma}$) of the 2 of 3 γ-ray signal from ortho-Ps decay to that of the 2 γ-ray signal from para-Ps decay remains nearly constant and then decreases rapidly indicating that ortho-Ps has a formation potential (i.e., like a work function except that Ps cannot exist within metals) of about 2 eV with respect to the aluminum scattering cell surface and consistent with a value deduced [2] for a "clean" aluminum surface. If ortho-Ps has a kinetic energy above 2 eV it breaks up at the surface and greatly increases the likelihood that the resulting positron will annihilate via two 511 keV γ-rays. Comparing the $R_{3\gamma/2\gamma}$'s obtained for O_2 and CO_2 with the $R_{3\gamma/2\gamma}$ for Ar versus positron energy above the Ps formation threshold provides evidence for Ps formation with inner orbital electrons [1]. The binding energies of the outermost inner orbital electrons deduced from these PsARS measurements are consistent with those determined by photoelectron spectroscopy. A most recent analysis indicates that a significant fraction (from 20 to 35%) of the Ps formed a few eV above the threshold for forming Ps with the outermost inner orbital electrons of O_2 and CO_2 is due to these inner orbital electrons. Several other PsARS investigations will be discussed, including the anomalous measured $R_{3\gamma/2\gamma}$ values at the Ps threshold for N_2 suggesting a possible attachment of the incident positron to N_2, and studies with different scattering cell surfaces and target gases.

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LOW-TEMPERATURE ANTIHYDROGEN-ATOM SCATTERING

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Recently the ATHENA and ATRAP groups at CERN managed to produce antihydrogen atoms at low temperatures [1]. Future goals of these experiments are to trap the antihydrogen atoms and perform spectroscopic measurements comparing antihydrogen with ordinary hydrogen. Such measurements can test the CPT theorem for baryons and leptons.

The new experimental progress has also stimulated interest in low temperature atom-antiatom collisions. Such collisions have several properties that make them qualitatively very different from ordinary atom-atom collisions. One obvious difference is that in the Coulombic nucleus-antinucleus interaction is *attractive*. Hence, the nucleus and antinucleus have a finite probability of overlapping in an atom-antiatom collision. Therefore it is necessary to include the strong nuclear force between the nucleus and antinucleus. The strong nuclear force leads both to annihilation processes and to a change in the elastic cross section.

I will discuss how the strong nuclear force may be incorporated in calculations of low-energy antihydrogen-atom scattering. In particular I will discuss a scattering-length method, which has been applied to antihydrogen-hydrogen and antihydrogen-helium scattering [2, 3, 5].

In addition to annihilation, antihydrogen-atom scattering can result in a number of collisional reactions such as elastic scattering, rearrangement to protonium and positronium, and even radiative association leading to formation of unusual short-lived atom-antiatom molecules. According to threshold laws inelastic processes will always dominate over elastic scattering at sufficiently low energies. I will present rates for the most important processes, with particular emphasis on the lowest energy (or temperature) at which elastic scattering dominates. This energy sets limits the possiblity of cooling antihydrogen via thermal contact with ordinary matter. I will also mention some of the theoretical difficulties connected with the rearrangement process.

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Creation and observation of the di-positronium molecule

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(ABSTRACT)

We have developed a multi-stage positron accumulator capable of delivering up to 10^8 positrons in a pulse with a temporal width (FWHM) of around 0.5 ns. This system is designed to deliver a large positron pulse with a short spatio-temporal extension such that the local positron density on the surface of a clean Al (111) target is high enough to allow the formation of di-positronium molecules. We report preliminary results.

ELECTRONIC EXCITATION OF H_2 BY POSITRON IMPACT

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In this work, we apply Schwinger Multichannel method (SMC) [1] to calculate the electronic excitation cross section of H_2 by positron impact. Specifically, we considered the $X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$, $X^1\Sigma_g^+ \rightarrow E, F^1\Sigma_g^+$ and $X^1\Sigma_g^+ \rightarrow C^1\Pi_u$ electronic transitions in the energy range from 13.5 to 30.0 eV.

In recent applications of SMC, the presence of spurious resonances was detected [2] in electronic excitation cross sections for N_2. These structures were generated by intrinsic problems with the basis set employed in the calculation. To overcome the problem, a technique based on direct comparison with the first Born approximation (FBA) was developed.

This procedure is called "Basis Set Born Approximation" (BSBA) because when correlation ($Q\hat{H}Q$) and Green's function ($VG_P^{(+)}V$) terms are switched off in the working expression for the SMC scattering amplitude, the results provided by the variational scattering basis set ($\{\chi_m\}$) should be identical to the FBA ones (nearly basis-set independent). The configurations weakly coupled to the scattering potential are then draw back until the BSBA cross section becomes similar to the FBA result.

In a first application of SMC to electronic excitation, the $X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$ electronic excitation of H_2 was considered in a "two state level of approximation" [3]. Due to the problems found in the works with N_2, the results presented before became uncertain. The main motivation for this work is to verify the reliability of the old results, and to verify the power of the BSBA technic to predict electronic excitation cross sections. In figure 1, we present the new results with the old ones and also with the experimental data o Sullivan *et al* [4]. We hope this work motivate experimentalists to realize new measurements with H_2 and other molecular targets in near future.

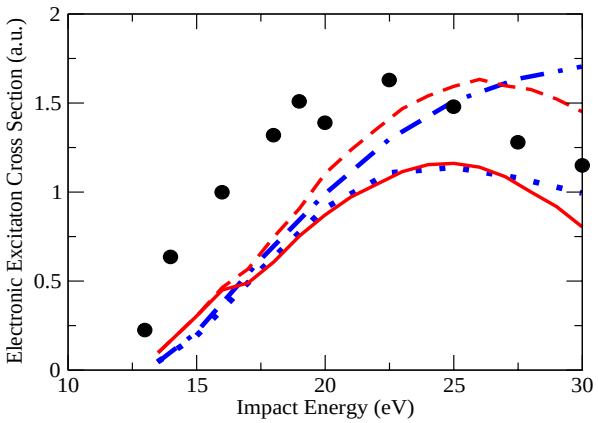

Fig. 1. $X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$ electronic excitation cross section. Circles: experimental data of Sullivan *et al.* [4]. Full line: old SMC results [3]. Dashed line: old Born-SMC results [3]. Line of points: new SMC results. Dashed-point line: new Born-SMC results.

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INNER SHELL IONIZATION BY POSITRON IMPACT

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Recently large discrepancies between experimental results and the values predicted by the binary encounter approximation theory and the atomic rearrangement theory have been reported for the In and Sn L x-ray production cross sections by electron impact in the energy range from near threshold to tens of keV [1].

In the present work, we have studied inner shell ionization by positron impact for Cu K-, Ag L-, In L- and Sn L-shells [2]. Development of an x-ray detector with thin Si(Li) crystals has enabled the measurements of the absolute cross sections in the energy range below 30 keV [3].

The determined values are plotted in figure 1 against the positron impact energy. Threshold behavior has been compared with the theoretical results calculated in the binary encounter formalism [4]. The values for the Cu K- and Ag L- shells have also been compared with the results in the plane wave Born approximation with Coulomb corrections [5]. The measured cross sections for the Cu K-shell are in good agreement with the theories. The results for the Ag, In, and Sn L- shells are, however, smaller than the theoretical calculations.

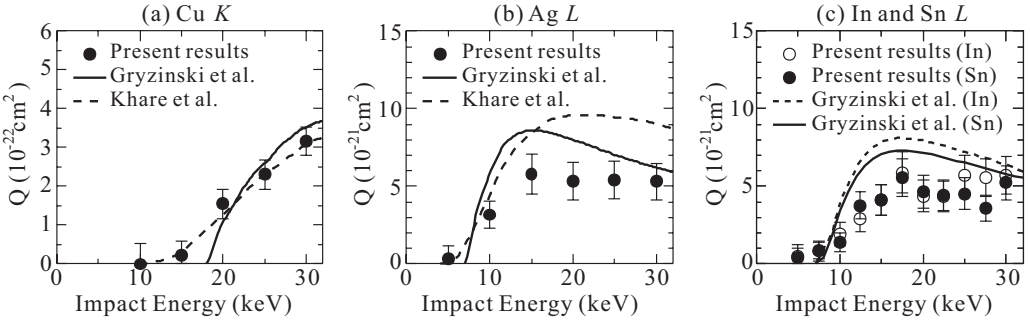

Figure 1: Inner shell ionization cross sections plotted against the positron impact energy. Theoretical results [4, 5] were also plotted.

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Positron physics in antihydrogen production - a look to the future

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The generation of large and dense positron plasmas have played a crucial role in the success of antihydrogen physics thus far. The ability in ATHENA to tailor-make the positron plasmas to the desired size and density [1], while being able to verify these plasma characteristics non-destructively in real-time [2], have contributed to a much better theoretical understanding of the detailed formation process [3]. However, in order to perform the high precision tests of the CPT theorem that is the goal of most efforts in the field, it will be necessary to trap the neutral antihydrogen atom in a multipole magnetic trap. There are now serious questions concerning the stability of non-neutral plasmas in the presence of such higher order magnetic fields, particularly as concerns quadropole fields [4]. I will briefly explain how we plan to overcome these problems in the new ALPHA experiment and also how plans to upgrade the Antiproton Decelerator resulting in an increase in antiproton number by a factor of 100 [5] might affect the dynamics of antihydrogen formation.

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Positron accumulation in ultra high vacuum with an electron plasma

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Various techniques for trapping positrons have been intensively developed in the last decades including slowing down via collisions with buffer gas [1] and by field ionization of Rydberg positronium atoms [2], etc., since such techniques are expected to open new fields of research.

We recently developed a new positron accumulation scheme, in which trapped electrons are used as an energy absorber for positrons [3]. The positron accumulation efficiency normalized by Na-22 positron source intensity is 10^{-5} (e^+/β^+), which is the result of several steps such as (1) solid Ne moderator efficiency to produce slow positrons(~0.2%), (2) transport efficiency of slow positrons into the trap (~50%), and (3) capturing efficiency of slow positrons in a trap (~1%).

We will discuss the present status and possibilities to further improve the efficiency.

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Positron and Positronium Interactions in Solids

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Positronium (Ps) in vacuum is a simple two-body system. It has been a topic of extensive experimental and theoretical investigation during the past several decades since the investigation of its properties allows for a very accurate test of QED. The lifetime, hyperfine splitting, and energy levels are now known with high accuracy.

In contrast, Ps in solids is a very complicated, many-body Coulomb interacting system. Our knowledge of the fundamental properties of Ps in solids is very limited because of theoretical and experimental difficulties.

In this talk we will focus on delocalized Ps state in $\alpha-SiO_2$, which was identified in the angular correlation of annihilation radiation (ACAR) spectrum more than thirty years ago[1]. The mean lifetimes of para-Ps and ortho-Ps in $\alpha-SiO_2$, however, have not been unveiled for many years. It has been impossible to resolve the para-Ps decay component from those due to ortho-Ps, positrons which do not form Ps (free positrons), and positrons trapped in lattice defects. The main reason for this is the instrumental limitations and small differences in the decay rates among these components.

Recently, we have succeeded in developing a new PAL spectrometer using a digital signal processing technique which has a high resolution in addition to high stability and a good signal-to-noise ratio[2]. We performed high-statistics measurements of the PAL spectra for $\alpha-SiO_2$ with this spectrometer, and determined the mean lifetime of para-Ps in $\alpha-SiO_2$. [3]

The lifetime of the para-Ps in $\alpha-SiO_2$ is found to be 156 ± 4 ps, which is much longer than its intrinsic lifetime of 125 ps. This indicates clearly that Ps in $\alpha-SiO_2$ is swollen. The average distance between the electron and positron in Ps becomes larger than its vacuum value, because of the screening of the Coulomb interaction between the constituent particles by electrons of the medium.

From this value and ACAR results for the identical sample, the electron-positron contact density κ is obtained to be $\kappa=0.34\pm0.01$. This value is in agreement with the results of the Zeeman mixing study[4], which suggests that a simple "two body picture" is valid. It is also valuable to compare this results with that of Time-Of-Flight measurements[5] and effective mass study[6].

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Modelling dynamical processes in molecular gases induced by low-energy positrons

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The availability of thermal or near-thermal positron sources have triggered in the last decade a tremendous development in the observation of processes that can occur in molecular gases once they interact with beams of these antiparticles over a broad range of low energies of chemical interest.

The processes of interest include elastic scattering, electronic and vibrational excitations, molecular ionization, positronium (Ps) formation and positron annihilation. One therefore needs to develop correspondingly articulate and flexible theoretical and computational tools that can successfully match the surprising variety of events, at the molecular level, which have been uncovered by the experiments.

In this talk I will endeavour to show a subset of examples which deal with polyatomic molecular gases and for which theory and computations have been able to provide realistic descriptions of the processes at hand. Thus, we will briefly show what can be gathered about vibrational excitation of small polyatomics (1), about the possible effects of nuclear motion on Protonation Affinities (2) and on the transient molecular deformation effects on annhilation processes (3).

I shall also try to show how one may carry out numerical "experiments" on hollow cages like C60, C20 or Cubane in order to assess the likelihood of trapping positrons inside such molecular cavities for realistic time periods (4,5), as has been found to occur for electron projectiles (6,7).

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NEW RESULTS ON POSITRON-MOLECULE ANNIHILATION, VIBRATIONAL FESHBACH RESONANCES AND BOUND STATES

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Positron trapping techniques have improved over the years allowing many scattering experiments that were previously not possible. One such advance is the use of a Penning-Malmberg buffer-gas trap and a solid rare-gas moderator to produce pulses of cold, monoenergetic positrons (~ 25 meV, FWHM). This cold beam was used to measure the first energy-resolved positron-on-molecule annihilation spectra [1,2]. Strong peaks in annihilation rate are observed at energies just below the vibrational modes of various molecules, such as alkanes (C_nH_{2n+2}). These peaks are due to vibrational Feshbach resonances (VFR) and provide evidence of positron-molecule binding.

It is presently unclear as to how various molecular features relate to positron-molecule binding and the magnitude of observed resonances in annihilation rate. To complicate matters, it seems that there are both global factors, which relate to all modes, and local factors, which relate to individual modes. For example, substitution of a single fluorine atom for a hydrogen in a large alkane reduces significantly the annihilation peaks associated with much of the vibrational mode spectrum, while the modes themselves are only marginally different [2]. We describe here the results of new experiments designed to further understand the global and local factors that determine positron-molecule binding and the annihilation resonances.

In this paper, the dependence on target morphology is studied for the ring hydrocarbons benzene, cyclohexane and cyclopropane. The spectra for these molecules are compared with those for alkanes (i.e., which are linear). Intriguing features of each comparison will be discussed. Results for halogenated methanes will also be discussed.

Since evidence indicates that the positron resonances are closely linked to the spectrum of vibrations, it is worth investigating the relative contribution of each type of mode to these resonances. Energy resolution limits our ability to distinguish between some modes in a single molecule, and so we examine collections of molecules which possess similar modes (e.g., ring molecules and halogenated methane molecules) in order to identify the modes responsible for VFR.

Also of interest is the extent to which simple, long-range electrostatic coupling can explain the magnitudes of the observed VFR. To address this, a comparison is presented of the annihilation and infrared-absorption spectra for various molecules. While some features in the IR and annihilation spectra are similar, it appears that this coupling alone cannot account for the observed annihilation spectra.

Finally, evidence is presented for a second, "positronically excited" bound state in the largest alkane molecules studied ($C_{12}H_{26}$, and $C_{14}H_{30}$). For these molecules, a second annihilation peak is observed slightly downshifted from the position of the C-H stretch mode. The energy at which this feature occurs is lower in the larger molecule, consistent with the previously observed result that the positron binding energy increases with molecular size.

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*In collaboration with L. D. Barnes, and C. M. Surko.

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Positron Binding Energies for Alkali Hydrides

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Abstract

Ab initio multireference single- and double-excitation configuration interaction (MRD-CI) calculations are carried out to study the interactions of positrons with the members of the alkali hydride class of molecules. A new computer program has been constructed for this purpose that makes use of the Table-Direct-CI method for construction of the required Hamiltonian matrices and electronic/positronic wave functions. The calculations indicate that the binding energy (positron affinity PA) of a single positron to these systems increases by an increment of 0.2-0.3 eV as the atomic number of the alkali atom is increased. It is found that the positron prefers a location in the more electronegative regions of such molecules, similarly as has been found in earlier calculations for the urea and acetone molecules. The positron orbital possesses a diffuse charge distribution with relatively small expectation values of the kinetic energy in all four systems considered. Each of the four positronic molecules is stable with respect to formation of either positronium (Ps) or HPs according to the present calculations. The potential curves of the latter systems are compared with their neutral counterparts and it is found that relatively large changes in the equilibrium bond distance of the hydrides occur as a result of the positron interaction. The importance of bond dipole moments in producing the binding of positrons to molecules is discussed, as well as the role that the electronegativity of the constituent atoms plays in determining the magnitude of the PA for a given system.

April 29, 2005

CALCULATIONS OF POSITRON INTERACTIONS WITH ONE- AND TWO-ELECTRON ATOMS

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A number of computational methods have, over the past decade, been successfully applied to the study of various positronic atoms [1]. We report here on the recent results from three different approaches; the configuration-interaction (CI) method, a hybrid CI-Kohn method, and the hyperspherical close-coupling (HSCC) method.

The CI method has become one of the most successful approaches towards solving positron-atom bound-state problems, but it suffers from slow convergence due to the presence of localised electron-positron pairing. Building on the study of Gribakin and Ludlow [2], we have used our CI and CI-Kohn calculations to examine the partial-wave convergence of positron-electron systems [3]. Armed with this knowledge, and recently parallelised computer code, we also present improved CI calculations of the alkali-metal positronic atoms [4]. Current CI (and other) estimates of the positronic atom binding energies are summarised in Figure 1.

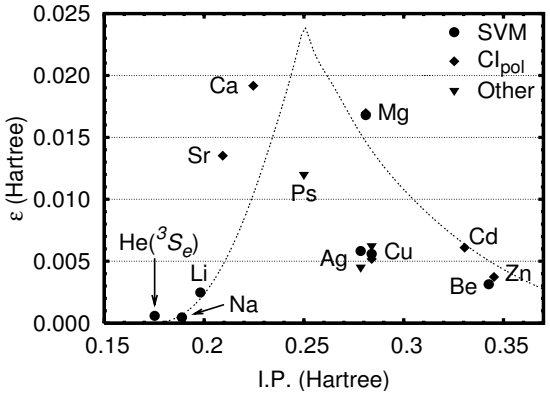

Fig. 1. Estimated binding energies of the known neutral atoms that bind a positron (c.f. Fig. 3 of Ref. [1]).

We also report on the results of HSCC calculations of positron scattering from both sodium and lithium in the low-energy range [5]. This was motivated by a recent experiment that measured the Ps-formation cross sections [6]. This experiment found strong disagreement with previous Ps-formation calculations [7, 8] for energies near and below 1 eV. Speculation arose in [6] that the calculations were not converged as sodium was later shown to be a positronic atom. Our results for sodium, as shown in Figure 2, find broad agreement with previous calculations and disagreement with the experimental data below 2 eV. The accurately-known $PsNa^+$ binding energy [1] is reproduced by our calculations, and hence, our low-energy results are reliable.

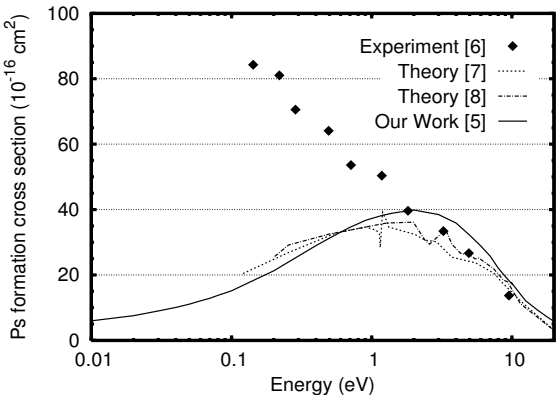

Fig. 2. Positronium formation cross sections for e^+-Na scattering (only the lower experimental limits of Ref. [6] are shown).

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LIST OF CONTRIBUTED PAPERS

Examination of quasi-bound states of $He\,\overline{p}$ and the possible existence of a bound state

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There is continuing interest in antihydrogen ($\overline{H}$) following the successful preparation of $\overline{H}$ by the ATHENA and ATRAP projects. See, for example, [1], [2]. $He\,\overline{p} + e^+$ is a rearrangement channel of $He + \overline{H}$. $He\,\overline{p}$ has been studied within the Born-Oppenheimer approximation. Using an approach similar to that of Jonsell *et al.* in their calculations for $H\overline{H}$ [3], the electronic energy curve of $He\,\overline{p}$ has been calculated using the variational method with basis sets containing up to 768 Hylleraas-type basis functions.

The energies and nuclear wave functions for 50 s states have been obtained from our potential by solving the nuclear wave equation numerically using the Cooley-Numerov algorithm. We intend to use the present calculations, along with entrance channel wave functions derived by a variational calculation by Armour *et al.* [4], to calculate cross sections for the $He + \overline{H} \rightarrow He\,\overline{p} + e^+$ rearrangement.

For the state with the lowest energy we calculate an energy, within the BO approximation, which is below the threshold for binding. However the competing effects of the BO approximation and the variational method will lower or raise slightly the calculated energy, respectively, when compared to the true energy value. If no bound state exists, $He\,\overline{p}$ has a quasi-bound state very close to the threshold for binding. The remaining states are all above the lowest continuum threshold for $He\,\overline{p}$ and are thus quasi-bound states.

For the low energy states of $He\,\overline{p}$ we find that the nuclei are so close together that is very like H^-.

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ENERGY APPROACH TO QED THEORY OF CALCULATION OF POSITRON IMPACT IONIZATION OF MULTIELECTRON ATOMS

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Considered will be processes, which lead to single (outer shell) ionization of the multielectron atom. Positron impact can lead to ionization via two reaction channels usually called break up (of the atom into an electron and ion) and transfer (of one atomic electron to the projectile to form positronium. The most accurate positron ionization cross sections for example, for helium are presented in [1] and analysed in comparison with that for electron impact ionization. Note that the features of particular interest are the merging of the cross sections above 600 eV when the first Born approximation is valid, the positron cross section exceeding the electron cross section at medium energies and a cross over of the cross section curves near threshold [1]. We suppose that a uniform theoretically comprehensive approach to the whole problem is needed. The most consistent approach to considered problems solving must base on the quantum electrodynamics (QED). In this paper the energy approach (gauge invariant formulation [2]) is used for consistent QED description of positron and electron collision (ionization) processes. As example we consider the positron impact ionization of He. We consider $a_{in}^{+}F_0$ as the initial state. In general form a scattered part for imaginary energy shift $ImdE$ appears at first in the second order of the atomic perturbation theory in the form of integral over the scattered positron energy e_{sc}: $de_{sc}G(e_{iv}, e_{ie}, e_{in}, e_{sc})/(e_{sc}-e_{iv}-e_{ie}-e_{in}-i0)$ with $ImdE=pG(e_{iv}, e_{ie}, e_{in}, e_{sc})$. Here e_{in} *and* e_{sc} are the incident and scattered energies respectively to the incident and scattered positron; G is a definite squired combination of the Coulomb and Breit inter particle interaction integrals [3]. We use further the optimized basis's of Dirac orbitals, which is got from minimization principle for contribution of the fourth QED perturbation theory diagrams to the imaginary part of energy shift, i.e., radiative width of atomic level [2]. Our atomic numerical code [2,3] is used. Preliminary results on positron impact ionization cross-section ($Å^2$) for helium are presented in table below and compared with results: A-Knudsen etal and B-Bielefeld (c.f.[1]).

Impact energy, eV	Measured/ A	Measured/ B	Calculated/ Present
50	0,23	0,29	0,24
100	0,52	0,45	0,51
200	0,45	0,40	0,46

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Positron Impact Ionization of water molecule

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The cross-sections for ionization and fragmentation of water are relevant in radiation damage and in the chemistry of planetary atmosphere. However, whilst data for electron-water interaction are available for a variety of processes [e.g. 1], measurements for positron-water interactions are very scarce [2, 3]. In particular, only an indirect estimation of Ps formation cross-section exist [4]. These observations triggered our recent investigation of water ionization by positron. The test run for direct ionization of Ar is compared with earlier data [5] and a good agreement with published results has been found. Thereafter, the direct ionisation cross-section for positron induced ionization of water has been measured for the first time. Total ionisation and Ps formation cross-section have been obtained. Finally, the double differential cross-section for water vapour has been also measured for the first time.

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Isomer Effect in Positron and Electron Scattering from C_3H_6 Molecules

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Hydrocarbons play an important role in high temperature plasmas in Tokamak fusion devices in plasma processing and many other fields [1], and have thus attracted research attention especially in electron scattering. Not only is a comparative study with positron impact invaluable in revealing more information of the scattering dynamics, but the positron and positronium impact physics is increasingly offering new areas of research interests [2].

In this work, total cross sections for the two stable isomers of the C_3H_6 molecules; propene [$H_3C{-}C{=}CH_2$] and cyclo-propane [*cyclic*($H_2C{-}CH_2{-}CH_2$)] are studied for the isomer effect owing to their characteristic differences in physical and chemical properties. The total cross sections (TCSs) measurements were carried out for 0.4-1000 eV electron and 0.2-1000 eV positron impact using a linear time-of-flight apparatus [3]. The Continuum Multiple Scattering (CMS) [4] calculations have also been performed for the theoretical analysis of the observed features in the TCSs. Some of the results obtained are shown in Fig. 1. Both TCSs are gradually decreasing below 2 eV, show the broad 4 – 40 eV peak split into two by a minimum at 10 eV for C_3H_6, and 13 eV for cyclo-C_3H_6, and gradually decrease above 30 eV. However, the isomer effect is clearly manifested in C_3H_6 TCSs being greater than cyclo-C_3H_6 TCSs in the range 2.2 – 25 eV by an average 18% and vice versa in the energy range 30 – 90 eV. Detailed comparative studies with the electron results will be presented at the conference.

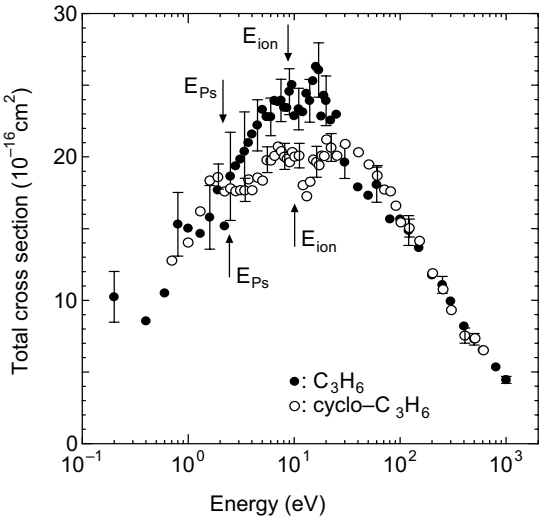

Fig. 1 C_3H_6 and cyclo-C_3H_6 positron TCSs. Arrows show the thresholds for ionization, E_{ion}, and positronium formation, E_{Ps}, i.e. pointing downwards for C_3H_6 and upwards for cyclo-C_3H_6.

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Positron and Electron Total Cross Sections for C_3H_6 and C_3F_6 Molecules: the Fluorination Effect

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Pure hydrocarbons play an important role for plasma diagnostics as impurities in Tokamak fusion divertor, as seed gases for production of radicals and ions in low temperature plasma processing [1]. On the other hand, fluorine-substituted hydrocarbons, the so-called perfluorocarbons (PFCs), are not the less important also as they play significant roles as reactive agents in plasma-assisted fabrication processes [2]. The hexafluoropropene ($F_3C{-}CH{=}CF_2$) molecule offers an opportunity for studying the effects of fluorine atom substitution on the electronic structure and spectra of propene ($H_3C{-}CH = CH_2$).

In this work, total cross sections (TCSs) for the two molecule were measured for 0.4-1000 eV electron and 0.2-1000 eV positron impact using a linear time-of-flight apparatus [3]. The Continuum Multiple Scattering (CMS) [4] calculations have also been performed to provide theoretical rationales to the observed features in the electron impact TCSs. Some of the results obtained are shown in Fig. 1. Among other features, the fluorination effect shows itself in the positron C_3H_6 TCSs being greater than the C_3F_6 results in the range 1.5 – 25 eV, with the difference averaging 30% in the peak region. Besides, these TCSs have a broad peak spanning the region 4 – 40 eV for C_3H_6, split into two by a minimum at about 10 eV, while this peak in C_3F_6 spans the even broader region of 4 – 200 eV and is split into three regions by the minima at about 10 eV and 70 eV.

These results will be discussed in greater detailed in comparison with the electron results at the conference.

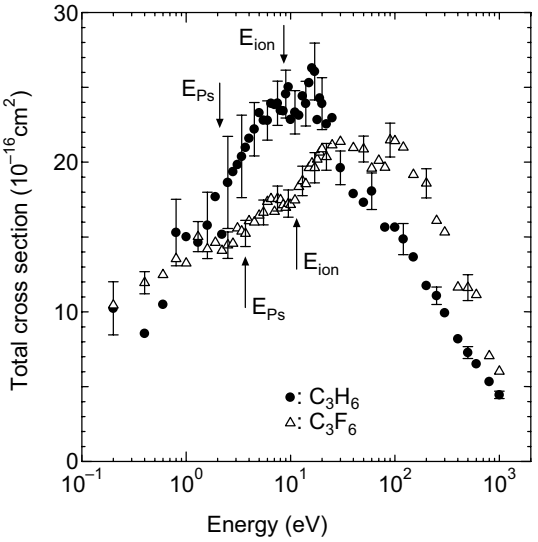

Fig. 1 C_3H_6 and C_3F_6 positron TCSs. Arrows show the thresholds for ionization, E_{ion}, and positronium formation, E_{Ps}, i.e. pointing downwards for C_3H_6 and upwards for C_3F_6.

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VIBRATIONAL RESONANCES IN POSITRON ANNIHILATION WITH KRYPTON DIMERS

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Experimental measurements of annihilation with a positron beam at high resolution (25 meV) [1, 2], have shown resonances in the annihilation rate parameter, $Z_{\rm eff}$, of alkane molecules. These can be explained by the capture of positrons into vibrational Feshbach resonances, which also account for very large values of $Z_{\rm eff}$ observed.

To examine the effect of vibrations on positron scattering and annihilation, we consider a simple model of Kr_2 dimer using the zero-range potential (ZRP) method. In the previous paper [3] the interaction between the atoms in the dimer was treated using the harmonic approximation (HA). This approximation does not describe well the true potential for weakly bound van der Waals molecules such as Kr_2. In this work we model the molecular interaction with the Morse potential (MP), $U(R) = U_{\rm min}[e^{-2\alpha(R-R_0)} - 2e^{-\alpha(R-R_0)}]$, whose parameters can be obtained from the known values of R_0, $U_{\rm min}$ and ω for the dimer.

The positron-molecule wavefunction outside the atoms can be written in the form of a linear combination with coefficients A_n and B_n,

$$\Psi = e^{i\mathbf{k}_0\cdot\mathbf{r}}\Phi_0(\mathbf{R}) + \sum_n A_n\Phi_n(\mathbf{R})\frac{e^{ik_n|\mathbf{r}-\mathbf{R}_1|}}{|\mathbf{r}-\mathbf{R}_1|} + \sum_n B_n\Phi_n(\mathbf{R})\frac{e^{ik_n|\mathbf{r}-\mathbf{R}_2|}}{|\mathbf{r}-\mathbf{R}_2|},$$

where $\mathbf{k}_0$ is the incident positron momentum, Φ_n is the nth vibrational state of the molecule, and $\mathbf{R} = \mathbf{R}_1 - \mathbf{R}_2$ is the interatomic distance. The two sums represent scattering events which leave the molecule in the nth excited state, and k_n is the corresponding positron momentum.

One can obtain a set of linear equations for the coefficients A_n and B_n, using the ZRP boundary condition. They can then be used to calculate $Z_{\rm eff}$ by the formula [3],

$$Z_{\rm eff} = Z_{\rm eff}^{(0)}\kappa_0^2\sum_n(|A_n|^2 + |B_n|^2),$$

where κ_0 is the zero-range parameter and $Z_{\rm eff}^{(0)}$ is the $Z_{\rm eff}$ value for an atom at zero positron energy.

For parameters $R_0 = 7.56$ a.u., $U_{\rm min} = 17.2$ meV and $\omega = 2.42$ meV, the bound states for MP are $\varepsilon_0 = -4.10$ meV and $\varepsilon_1 = -1.45$ meV, whereas for HA they are $\varepsilon_0 = -4.51$ meV, $\varepsilon_1 = -2.30$ meV and $\varepsilon_2 = -0.11$ meV. So in MP we find a smaller binding energy than in HA. We also see that MP results in a greater vibrational frequency for the e^+Kr_2 complex than that of Kr_2, whereas HA suggests it to be less.

Figure 1 shows $Z_{\rm eff}$ for both approximations. Though the resonances are in different positions, the strength of the first resonance ($n = 2$ for MP, $n = 3$ for HA) remains almost the same. After thermal averaging of $Z_{\rm eff}$ over the Maxwellian positron energy distribution, the graphs of $\bar{Z}_{\rm eff}(T)$ for MP and HA become similar, with the resonance contribution being about an order of magnitude greater than the background.

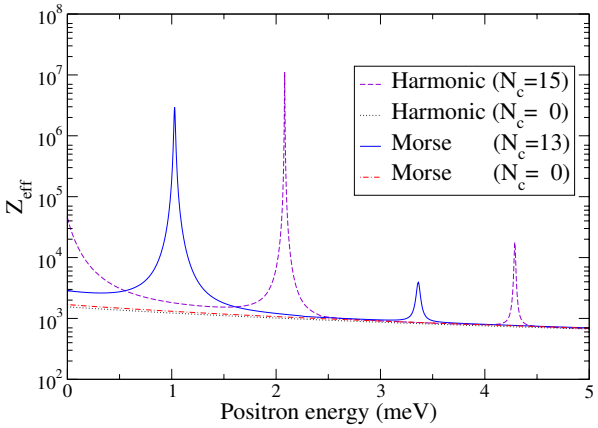

Fig. 1. Comparison of $Z_{\rm eff}$ for MP and HA, calculated using vibrational states with $n \le N_c$. $N_c = 0$ corresponds to the fixed nuclei approximation.

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Study of Atomic Clusters and Nanoparticles Using Positron Scattering and Annihilation Techniques*

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This paper discusses the potential use of positron scattering and annihilation techniques to study clusters and nanoparticles, *in situ, in vacuo*. Possible studies include the use of high-resolution (e.g., 25 meV) scattering techniques to study cluster size and electronic and vibrational excitations [1]; the use of positron annihilation and positronium atom formation to probe electronic structure, study fragmentation, and form specific cations [2,3]; and the use of positron-induced Auger spectroscopy to study surface properties. Phenomena of interest include trapped-positron states in C_{60} and similar caged structures and the fragmentation of polycyclic aromatic molecules.

* This work is supported by the U. S. National Science Foundation and Army Research Office.

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A Multicell trap for Long-term Confinement of Large Numbers of Positrons*

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There are numerous potential applications of high-capacity and/or portable antimatter traps [1]. Previously, we proposed the design for a high-capacity, multicell Penning-Malmberg trap for positrons [1, 2]. Here, we discuss an improved design based on the results of recent experiments [3] to confine and tailor electron plasmas using the "rotating wall" (RW) technique. We are now able to access a regime in which careful tuning of the RW frequency is unnecessary, and transport is insensitive to plasma density and length [3]. Operating a high-capacity, multicell positron trap in this regime offers a number of advantages. The design of a 95-cell trap for $N \geq 1 \times 10^{12}$ positrons will be discussed. Directions for future work, including possible extensions of this design and practical limits on positron accumulation, will be discussed.

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Single-component Plasma Compression with Application to Positron Plasmas*

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The application of a rotating electric field to plasmas confined in Penning-Malmberg traps [i.e., the so-called "rotating wall" (RW) technique] has been used extensively to radially compress and increase the confinement of single-component electron, positron, and ion plasmas [1]. We describe here the results of experiments demonstrating a robust operating regime in which compressed, torque-balanced steady states can be achieved over a broad range of RW frequencies without the need to tune to a plasma mode [2]. The current experiments are done on electron plasmas. Plasmas can be driven into a regime in which the transport is roughly independent of density. The RW heating is balanced by cyclotron cooling in a 5T magnetic field. A key result is the discovery that the plasma density increases until the central $E \times B$ rotation frequency matches the frequency of the applied RW field. An emerging physical model of the resulting torque-balanced steady states will be discussed. The implications of these results for the ultimate limits on single-component positron plasma confinement and cold, bright beam formation will also be discussed.

*This work is supported by the U. S. National Science Foundation.

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DIFFERENTIAL CROSS SECTIONS FOR FRAGMENTATION OF POSITRONIUM

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In a recent experiment [1] the longitudinal energy distribution of the ejected positron from positronium (Ps) ionization in Ps(1s)+He(1^1S) collisions has been measured. The measurements have been made at energies of $\leq$33eV where excitation of the He(1^1S) is either impossible or very unlikely. Consequently, we need only concentrate upon collisions in which the atom remains unexcited. Here, we report impulse approximation (IA) calculations for the process.

If the ejected positron has a velocity $\mathbf{v_p}$ making an angle θ_p with respect to the incident direction, then its longitudinal energy is $E_{pl} = E_p \cos^2\theta_p$ where $E_p = \frac{1}{2}v_p^2$ is the total energy of the positron. The measured cross section is then

$$\frac{d\sigma}{dE_{pl}} = \frac{d\sigma^+}{dE_{pl}} + \frac{d\sigma^-}{dE_{pl}} \tag{1}$$

where $d\sigma^{\pm}/dE_{pl}$ is given by

$$\frac{\pi}{\sqrt{E_{pl}}}\int_{E_{pl}}^{E_m}\frac{d^2\sigma}{dEd\Omega_p}\left(E_p, \cos\theta_p = \pm\sqrt{\frac{E_{pl}}{E_p}}\right)\frac{dE_p}{\sqrt{E_p}} \tag{2}$$

The experiment collects positrons ejected into both the forward (+) and backward (-) scattering cones. In (2) $d^2\sigma/dEd\Omega_p(E_p, \cos\theta_p)$ is the double differential cross section (DDCS) with respect to the positron energy and ejection angle, and E_m is the maximum energy available to the emitted positron. The DDCS is obtained by integration of the triple differential cross section $d^3\sigma/dEd\Omega_e d\Omega_p$ over the angles of the ejected electron.

In our IA, and in atomic units,

$$\frac{d^3\sigma}{dEd\Omega_e d\Omega_p} = \frac{v_p v_e}{4v_0}\left|f^{IA}\right|^2 \tag{3}$$

where

$$\begin{aligned} f^{IA} &= 2\langle\phi^-_{\boldsymbol{\kappa}}(\mathbf{t}) \mid e^{-i\mathbf{q}\cdot\mathbf{t}/2} \mid \phi_a(\mathbf{t})\rangle f^+_{el}(\bar{v}^+, q) \\ &\quad +2\langle\phi^-_{\boldsymbol{\kappa}}(\mathbf{t}) \mid e^{i\mathbf{q}\cdot\mathbf{t}/2} \mid \phi_a(\mathbf{t})\rangle f^-_{el}(\bar{v}^-, q) \\ \boldsymbol{\kappa} &= \frac{1}{2}(\mathbf{v_p} - \mathbf{v_e}) \\ \mathbf{q} &= 2\mathbf{v_0} - \mathbf{v_p} - \mathbf{v_e} \\ \bar{v}^+ &= \mathrm{Max}\left(\mid 2\mathbf{v_0} - \mathbf{v_e} \mid, v_p\right) \\ \bar{v}^- &= \mathrm{Max}\left(\mid 2\mathbf{v_0} - \mathbf{v_p} \mid, v_e\right) \end{aligned} \tag{4}$$

In (3) and (4) $\mathbf{v_0}$ is the velocity of the incident Ps(1s) and $\mathbf{v_p}(\mathbf{v_e})$ is the velocity of the ejected positron (electron). In (4) $f^{\pm}_{el}(\bar{v}, q)$ is the amplitude for elastic scattering of a free positron (+)/ electron (-) by the atom, where the positron/electron is incident with speed $\bar{v}$ and scattered with momentum transfer of magnitude q. The amplitude $f^+_{el}(f^-_{el})$ has been calculated in the static (static-exchange) approximation. The wave functions $\phi_{1s}(\phi^-_{\boldsymbol{\kappa}})$ represent the initial 1s state (final ionized state) of the Ps.

We shall report results calculated using (4) at the conference.

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IONIZING COLLISIONS BY POSITRONS WITH He AND CO_2

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Abstract

Ionization of an atom or molecule by positron impact can occur via a number of channels: annihilation ($e^+ + A \rightarrow A^+ + 2\gamma$), Positronium formation ($e^+ + A \rightarrow A^+ + Ps$) and direct ionization ($e^+ + A \rightarrow A^+ + e^+ + e^-$). Recent detailed measurements of the total ionization cross-section, encompassing all of the above processes, for ($Q_i^t(He)$) from threshold up to 850eV have been performed [1]. In conjunction with available data for the direct ionization cross-section ($Q_i^+(He)$), these allow the extraction of the Positronium formation cross-section [2] ($Q_{Ps}(He)$) according to:

$$Q_{Ps} = Q_i^t - Q_i^+ \qquad (1)$$

Comparisons with available theoretical and experimental results reveal some discrepancies which will be discussed at the workshop.

The investigation is currently being extended to Carbon Dioxide, with particular attention given to the simultaneous process of Positronium formation with an ionic excitation [3], i.e,

$$e^+ + CO_2 \rightarrow Ps + CO_2^{+*}.$$

This process is being studied in detail by measuring ion fragment – photon coincidences and the energy dependence of the cross-section for this simultaneous process ($Q_{sim}(CO_2)$) is reported. Total ionization cross-section ($Q_i^t(CO_2)$) is being measured at the same time. From these and additional measurements of $Q_i^+(CO_2)$, $Q_{Ps}(CO_2)$ will be extracted according to (1) above and preliminary results will be presented at the workshop.

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An Intense Slow Positron Production for 15 MeV LINAC at Argonne National Laboratory

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Abstract

An intense slow positron beam using a 20 MeV LINAC (average current 1.25 x 10^{15} e^-/s) at the Radiation and Photochemistry group, Chemistry Division of Argonne National Laboratory (ANL) has been proposed and studied. Computer simulated results by optimizing the positron yield and distribution of energy and angle show that a slow positron production at 10^{10} e^+/s is promising. A proposed design of intense slow positron beam with optimal conditions of incident electron/converter configuration, moderation, and extraction/transportation will be presented.

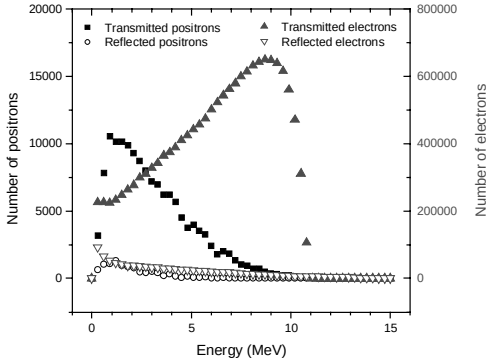

Figure 1 Simulated positron and electron energy distributions for 2 mm Ta converter for 10^6 e^- from LINAC at the normal incident angle .

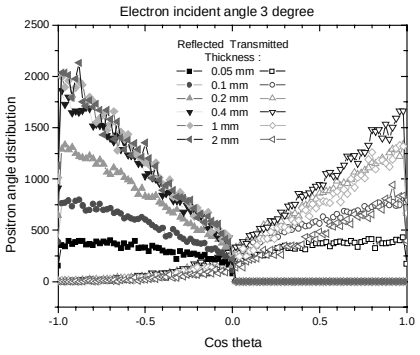

Figure 2 Simulated positron angle distribution at different thickness of Ta converter for incident angle= 3º.

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CALCULATIONS OF CROSS SECTIONS FOR VERY LOW-ENERGY HELIUM-ANTIHYDROGEN SCATTERING

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The ATHENA and ATRAP projects are continuing their work on antihydrogen at CERN after their successful preparation of antihydrogen in 2002. See, for example, [1,2]. We have already carried out calculations of cross sections for very low-energy hydrogen antihydrogen ($H\bar{H}$) scattering [3,4].

There is currently considerable interest in the interaction of helium with antihydrogen both as a possible means of cooling $\bar{H}$ and as a way of determining the $\bar{H}$ loss rate due to the presence of He as an impurity. We are in the process of carrying out calculations of very low-energy cross sections for $He\bar{H}$ scattering. We have calculated wave functions and energies for $He\bar{H}$ in the Born–Oppenheimer approximation using basis sets that contain Hylleraas-type functions [5]. These calculations give accurate results for the energy but not as accurate as the values obtained by Strasburger and Chojnacki using a basis set made up of explicitly correlated Gaussian functions [6].

Thus we used Strasburger and Chojnacki's energy values to obtain the potential that we required to calculate elastic scattering cross sections. We have used our wave functions to calculate the delta-function expectation values that determine the positron-electron annihilation rate into gamma rays. We have also used them to calculate cross sections for rearrangement processes using the distorted wave T-matrix approach used by Jonsell et al. in their calculations on $H\bar{H}$ [4].

Results will be presented at the conference for the antiprotonic He + Ps channel. A progress report will be given on calculations on the $He\,\bar{p}+e^+$ channel. In addition, it is hoped to be able to report on preliminary work on the $\alpha\bar{p}+Ps^-$ channel.

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ANTIPROTON ANNIHILATION IN LOW-ENERGY ANTIHYDROGEN SCATTERING BY SIMPLE ATOMS AND MOLECULES

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The ATHENA and ATRAP projects are continuing their work on antihydrogen at CERN after their successful preparation of antihydrogen in 2002. See, for example, [1,2]. We have already carried out calculations of cross sections for very low-energy hydrogen antihydrogen ($H\bar{H}$) scattering [3] but this did not take into account antiproton annihilation.

Antiproton annihilation in what would otherwise be elastic scattering is brought about by the strong interaction and the cross section for it is thus much larger than for positron-electron annihilation, which is brought about by the electromagnetic interaction. Experimentalists would like to have more information about it to be able to understand its role in bringing about loss of $\bar{H}$.

Recently, we carried out calculations of antiproton annihilation cross sections for $H\bar{H}$ scattering [4] using the complex potential of Kohno and Weise [5] to represent the strong interaction between the proton and the antiproton. This is a largely phenomenological potential but it takes into account the isospin invariance of the strong interaction and effects due to the singlet or triplet spin state of the nuclei.

The results we obtained for the annihilation cross section and the change in the elastic cross section due to the strong interaction are similar at very low energies to the results obtained by Jonsell *et al.* [6] by a scattering length calculation using the effective range expansion method of Trueman [7]. They are significantly smaller than the values obtained by Voronin and Carbonell [8] using a coupled channel method and a complex strong interaction potential.

We are in the process of calculating antiproton annihilation cross sections and the change in the elastic cross section for very low-energy $He\bar{H}$ scattering using a complex potential. A scattering length calculation by Jonsell *et al.* [9] indicates that the annihilation cross section is significantly larger than in the case of $H\bar{H}$. It is important that this result should be confirmed as a high annihilation cross section is likely to give rise to unacceptable loss of $\bar{H}$ if ultra-cold He is used to cool $\bar{H}$. We will report on this at the conference.

As the high annihilation cross section value obtained by Jonsell *et al.* casts doubt on the possibility of using He to cool $\bar{H}$, attention is turning to H_2. We hope to be able to present preliminary results for $H_2\bar{H}$ at the conference.

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Statistical analysis of the Doppler Broadening coincidence spectrum of the Electron-Positron Annihilation Radiation in Aluminum

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Positron annihilation spectroscopy is a well-established technique and has been extensively utilized to probe condensed matter systems [1]. With the incorporation of a second Ge detector to measure both annihilation photons [2], the Doppler Broadening Spectroscopy undergoes a great improvement, with a gain of $\sim\sqrt{2}$ in the relative energy resolution of the two detectors for the observation of the annihilation peak, and a great reduction of the background. Other important aspect, that does not receive much attention, is that in this coincidence measurement one obtains a two-dimensional spectrum in energy (Doppler-broadening coincidence spectrum), where the phenomena related to annihilation and those to the acquisition system are distributed through the spectrum. Then, one can distinguish these effects quite clearly. With the goal of treating all of these phenomena, we accomplished a statistical treatment for the Doppler broadening coincidence spectrum [3, 4, 5]. The Doppler-broadening coincidence spectrum was modeled by a two-dimensional function that was fitted, after convolution with the response function of the detector system, to an experimental spectrum. The obtained reduced chi-square value was 1.11. The relative intensities of positron annihilation with conduction band was 94.0 (3)%, with the 2p shell electrons was 5.7(3), with the 2s electrons was 0.29(16), with 1s electrons was 0.0126(13), in-flight positron annihilation was 0.064(3). The three Fermi cutoff parameters resulted 6.758 (9), 10.013 (11), and 15.532(10), expressed in 10^{-3} m_0c units. We have found that a complete analysis of the Doppler-broadening coincidence spectrum of the annihilation radiation is possible, in this case. Differently from the usual approach, this procedure allows the determination of data uncertainties. Thus, hypotheses can be tested and different results can be averaged.

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ELECTRONIC EXCITATION OF CO BY POSITRON IMPACT

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The development of high resolution ($\Delta E \sim 25$ meV FWHM) beam of positrons using the highly efficient buffer–gas positron accumulation technique (modified Penning-Malmberg trap) has opened up a new era in the study of positron physics [1, 2, 3]. The bright low–energy monochromatic positron beam allows experimentalists to perform highly sophisticated scattering experiments where measurements of state–resolved absolute cross sections for electronic or vibrational excitations are possible.

We report in this conference differential and integral cross sections for the electronic excitation of carbon monoxide CO by positron impact. The calculations were carried out with the Schwinger multichannel method (SMC), and the formal aspects of this approach are discussed in detail elsewhere [4, 5]. In these calculations, we included six–channel, namely the excited A $^1\Pi$, I $^1\Sigma^-$ and D $^1\Delta$ states, and the ground state X $^1\Sigma^+$. We expected to find a resonant feature in the excitation cross section of the A $^1\Pi$ state, consistent with the experimental $a\ ^1\Pi_g$ excitation cross section of the isoelectronic nitrogen molecule [2]. Our *ab initio* e^+–CO scattering calculation did not reproduce the conpicuous resonant-like structure, being consistent with previous e^+–N_2 scattering calculations [6, 7]. It could be claimed that present calculation do not take nuclear motion and the positronium formation channel into account. The scattering amplitudes were improved by combining the SMC approach ($l \leq 2$) with the first Born approximation (FBA) ($l \geq 3$) for the A $^1\Pi$ and D $^1\Delta$ states. The I $^1\Sigma^-$ state was calculated only with the SMC approach ($l \leq 5$) since the FBA does not contribute to the SMC.

In Fig. 1, we present integral excitation cross sections to the A $^1\Pi$ state and his partial cross sections.

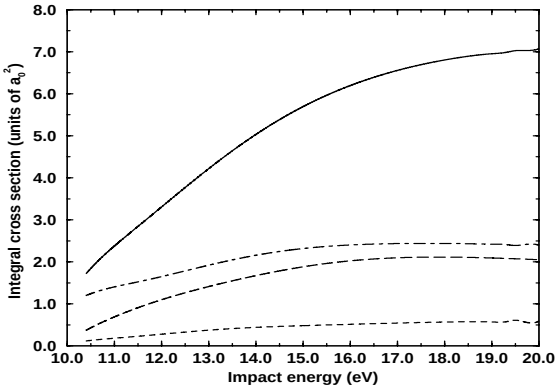

Fig. 1. Integral cross section for the electronic excitation to the A $^1\Pi$ state of CO by positron impact. Solid line: Total cross section (summed over all symmetries). Also shown are the partial cross sections. Short dashed line: $^2\Sigma$ symmetry; dot–dashed line: $^2\Pi$ symmetry; long dashed line: $^2\Delta$ symmetry.

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POSITRONIUM IMPACT ON LITHIUM

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We investigate positronium (Ps) scattering by lithium (Li) using a coupled pseudostate approximation and a model potential one - electron description of the Li atom. The collisional wave function, Ψ, is expanded as

$$\Psi = \sum_{a,b} \Big[G_{ab}(\mathbf{R}_1)\phi_a(\mathbf{t}_1)\psi_b(\mathbf{r}_2) + (-1)^{S_e} G_{ab}(\mathbf{R}_2)\phi_a(\mathbf{t}_2)\psi_b(\mathbf{r}_1) \Big] \quad (1)$$

where $\mathbf{r_p}(\mathbf{r_i})$ is the position vector of the positron (ith electron) relative to the Li nucleus, $\mathbf{R_i} = (\mathbf{r_p} + \mathbf{r_i})/2$, $\mathbf{t_i} = \mathbf{r_p} - \mathbf{r_i}$, the sum in (1) is over Ps states ϕ_a and Li valence orbital states ψ_b, and S_e (=0, 1) is the total electronic spin of the system.

The valence states of Li have been generated using the model potential of Stein [1]. We are interested in collisions involving 2s and 2p states of Li. However, the potential of Stein also supports an unphysical 1s state. We have found that omission of this state in the approximation (1) can lead to pronounced unphysical structures in the physical Ps - Li cross sections. Accordingly, we include all three Li states, 1s, 2s, 2p, in (1). We would expect this to give reasonable results provided that cross sections between the physical 2s and 2p states and the unphysical 1s state are small, which they are.

For the Ps states in (1) we have used a nine element set, 1s, 2s, $\overline{3s}$, $\overline{4s}$, 2p, $\overline{3p}$, $\overline{4p}$, $\overline{3d}$, $\overline{4d}$ where states denoted by a 'bar' are pseudostates. The pseudostates help us to represent the ionization of Ps in a discrete way. Substituting (1) into the Schrodinger equation and projecting with $\phi_a(\mathbf{t_1})\psi_b(\mathbf{r_2})$ leads to coupled equations for the functions $G_{ab}(\mathbf{R})$. These have been reduced to partial wave form and solved using the R- matrix technique.

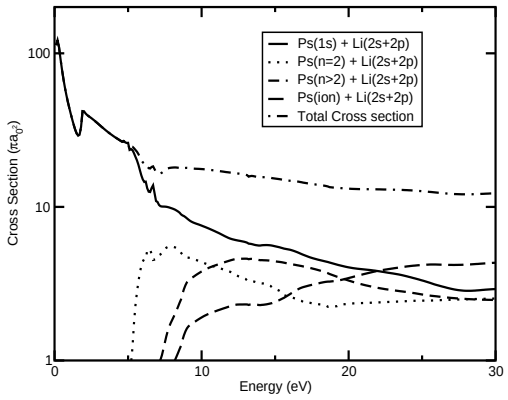

Figure 1

Figure 1 shows what happens to the Ps irrespective of the final state of the Li atom.

More detailed results will be presented at the Conference.

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IONIZATION OF HELIUM BY ANTIPROTONS

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We report the single ionization cross section for $\bar{p}$ - He collisions using a single centre coupled state approximation [1] where the electron wave function is expanded in terms of a B-spline basis. The relevance of B-splines in the present situation is their ability to represent the continuum (ionizing) channels accurately.

Theory

We assume that the $\bar{p}$ moves along a straight line trajectory, $\mathbf{R} = \mathbf{b} + \mathbf{v}t$, with $\mathbf{b}$ the impact parameter, $\mathbf{v}$ the impact velocity and t the time. We adopt an independent electron model of the atom. For each electron in He the Schrodinger equation is written, in atomic units, as

$$(H_{IP} + V_{int} - i\frac{\partial}{\partial t})\Psi(\mathbf{r},t) = 0 \qquad (1)$$

where $\mathbf{r}$ is the position vector of the electron with respect to the atomic nucleus. The atomic Hamiltonian (H_{IP}) is given by

$$H_{IP} = -\frac{1}{2}\bigtriangledown^2 + V_{eff}(r)$$

and

$$V_{int} = \frac{1}{|\mathbf{r} - \mathbf{R}|}$$

is the time dependent interaction between the projectile and the target electron. The effective potential V_{eff}(r) is of the form

$$V_{eff}(r) = -\frac{q}{r} - \frac{exp(-\lambda r)}{r}(a + br)$$

where $a = (Z-q)$=1, with $Z = 2$ and $q = 1$ being the nuclear and asymptotic charges of the He^+ ion. The two arbitrary parameters b and λ are are taken to be b= 0.502 and $\lambda = 2.51$. This gives a 1s orbital binding energy -0.9031 au which is close to the ionization potential -0.904 au of the He atom.

The total wave function is expanded as

$$\Psi(\mathbf{r},t) = \sum_{nlm} a_{nlm}(t)\phi_{nlm}(\mathbf{r})exp(-i\varepsilon_{nl}t), \qquad (2)$$

where $\phi_{nlm}(\mathbf{r})$ is given by

$$F_{nl}(r)[(-1)^m Y_{lm}(\mathbf{r}) + Y_{l-m}(\mathbf{r})]/\sqrt{2(1+\delta_{m,0})}.$$

The radial part of the wave function $\phi_{nlm}(\mathbf{r})$ is further expanded as

$$F_{nl}(r) = \sum_i c^l_{ni}\frac{B^k_i(r)}{r}$$

where the B^k_i(r) are k-th order B-spline functions.

Using (1) and (2) we obtain coupled equations for the expansion coefficients $a_{n'l'm'}(t)$,

$$i\frac{d}{dt}a_{n'l'm'}(t) = \sum_{nlm} exp[i(\varepsilon_{n'l'} - \varepsilon_{nl})t]V_{n'l'm',nlm}a_{nlm}(t)$$

where $V_{n'l'm',nlm} = < \phi_{n'l'm'}|V_{int}|\phi_{nlm} >$. These are solved with respect to the initial conditions: $a_{n'l'm'}(-\infty)=\delta_{n'l'm',1s}$. The sum of the probabilities $P_{nlm}(b) = |a_{nlm}(\infty)|^2$ over states ϕ_{nlm} with positive energies ϵ_{nl} gives the ionization probability for a particular impact parameter. The single ionization cross section of He in the so called independent particle model (IP) is then given by

$$\sigma = 2\pi\int_0^\infty 2P(b)(1-P(b))bdb,$$

where

$$P(b) = \sum_{nlm,\epsilon_{nl}>0} P_{nlm}(b).$$

Results will be presented at the Conference.

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Abstract for Poster:

Positronium Scattering Cross-Sections

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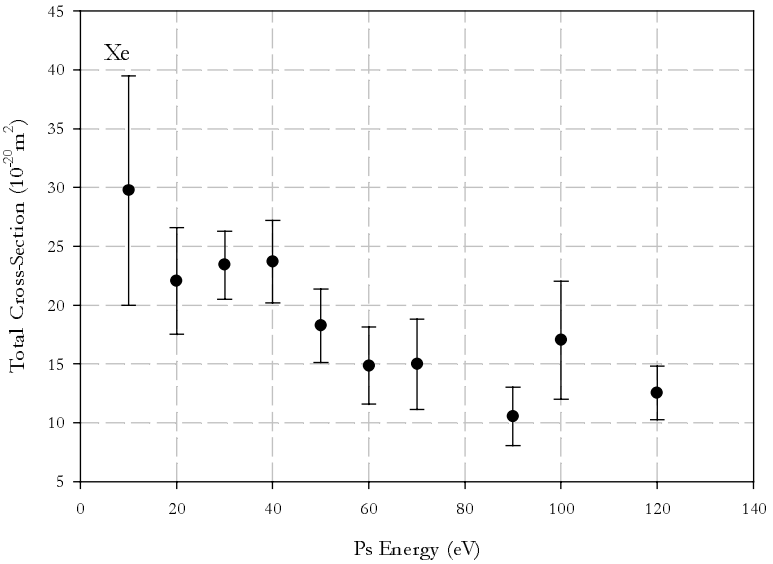
The results of recent investigations of Positronium interactions with simple atoms and molecules will be presented.

The total cross section σ_T for orthopositronium (o-Ps) scattering from various molecular (i.e. N_2 [1], H_2O [2], O_2 [2]) and noble (i.e. Ne [3] and Xe [3]) gases have been measured using a variable energy o-Ps beam in the range 10-250eV. These results will be presented at the workshop and compared with results from different targets [4,5] and corresponding cross- sections of electrons and positrons. Preliminary results for Xe are shown below.

This work is supported by the European Union (EPIC network grant. No. HPRN 00179) and the- Engineering and Physical Science Research Council UK (grant No GR/S16041/01*).*



[1] D E Leslie, S Armitage, J E Beale, G Laricchia, in preparation
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Recent Measurements of Low Energy Positronium-Gas Scattering using Age-Momentum Correlation

A new Age-Momentum Correlation apparatus has been built for the purpose of studying Positronium-Gas scattering. This apparatus uses a HPGe detector to perform time-resolved Doppler Broadening Studies on positronium in a gas environment. With this information, energy as a function of time since positronium formation can be extracted and used to calculate a momentum transfer cross-section. This method has significantly improved both data rate and energy resolution over previous measurements that also used Doppler broadening methods. More importantly, the simultaneous acquisition of both time and energy spectra allow for systematic checks that were not available to previous experiments. Recent results will be presented.

Potential Energy Curves for the Interaction of a Positron with Noble Gas Atoms

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Treating a positron as a light nucleus and the complex positron-atom within the quasi-molecule approximation [1], we have obtained adiabatic potential energy curves for its scattering by the He and Ne atoms. Different elastic and inelastic processes that contribute to the total scattering cross section are then rationalized in standard molecular terms of dissociation and nonadiabatic couplings. The procedure is extensible to other atoms and hopefully to molecules.
Supported by CNPq, Capes and Fapemig

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The Australian Positron Beamline Facility

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[2]*Flinders University, Australia*

A new positron beamline facility has been constructed to take advantage of the opportunities presented by the development of buffer gas trap technology. The basis of the beamline is a two-stage Surko trap which uses combined magnetic and electrostatic fields and a buffer gas of N_2 and CF_4 to trap positrons and cool them to room temperature [1]. The room temperature positrons can then be used as a reservoir to form a pulsed, high-resolution positron beam for use in low energy scattering studies [2].

The first stage of the apparatus is a commercially available unit purchased from First Point Scientific Inc. and provides a neon moderator for use with a ^{22}Na positron source. The beam from this first stage is then directed to the second stage, containing a buffer gas trap, where it is trapped and cooled. The trap incorporates a segmented electrode to provide a rotating electric field, allowing radial compression of the trapped cloud of positrons [3]. By careful manipulation of the trap electric fields, a pulsed beam is formed to be used in experiments. An energy resolution of 25 meV or less should be attainable using this system. After the trap, the positron beam will be directed to one of two experimental stages, for studies of atomic and molecular physics or materials science. The atomic and molecular physics apparatus is currently under construction and should come on line in the latter half of 2005.

Techniques that allow the measurement of scattering cross sections in a high magnetic field (~500 gauss) will be employed to study positron scattering processes at a level of detail that has been unobtainable until recently [4]. Additionally, the beamline will be used to study electron scattering, providing a valuable way to check the operation of the apparatus by comparing measurements with well known electron scattering standards. Electron scattering studies will also make measurements of total inelastic cross sections for processes such as vibrational and electronic excitation, which have been notoriously difficult using conventional electron scattering techniques. The first target to be examined in the new apparatus will be helium, with the goal of establishing new benchmark measurements for comparison with state of the art theoretical predictions. Very low energy (<1 eV) differential elastic cross sections will be measured, as well as discrete excitation cross sections, a first for positron scattering from helium.

Details of the construction and operation of the first two stages of the experiment will be presented as well the design and plans for the experiments in atomic and molecular physics.

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MANY-BODY THEORY OF GAMMA SPECTRA FROM POSITRON-ATOM ANNIHILATION

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During annihilation of the positron with an electron, two gamma rays are emitted. Information contained in these rays can be used to study the electronic environment around the annihilation site. This information is unique to each atom, and can be used, in particular, to identify annihilation sites in molecules [1].

The gamma rays carry away the energy of the two particles, $E \approx 2mc^2$, and their total momentum, $\mathbf{P}$, is equal to the momentum of the electron-positron pair. The distribution of these momenta leads to the following spectrum of energies E_γ of the gamma quanta,

$$w(\epsilon) = \frac{4\pi}{c} \sum_n \int_{2|\epsilon|/c}^{\infty} |A_n(\mathbf{P})|^2 \frac{PdP}{(2\pi)^3}, \qquad (1)$$

where $\epsilon = E_\gamma - mc^2$, and $A_n(\mathbf{P})$ is the amplitude of annihilation for the electron orbital n. Using many-body theory, this amplitude can be represented as the following set of diagrams:

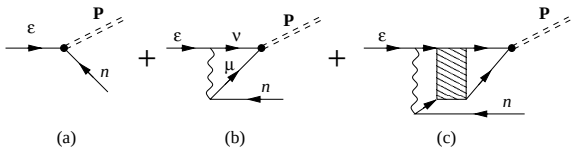
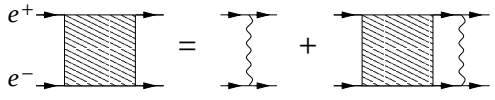


Fig. 1. ε is the incident positron, n is the hole, ν and μ are intermediate positron and electron states, wavy lines represent Coulomb interactions, and double dashed lines describe γ-quanta.

The shaded block in diagram (c) of Fig. 1 is the sum of the electron-positron ladder diagram series, known as the electron-positron vertex function. It is found from the linear equation [2]



In the lowest order, the amplitude is given by

$$A_{\nu\epsilon}(\mathbf{P}) = \int e^{i\mathbf{P}\cdot\mathbf{r}} \psi_n(\mathbf{r}) \varphi_\varepsilon(\mathbf{r}) d\mathbf{r} \equiv \langle 2\gamma\mathbf{P}|\delta|n\varepsilon\rangle \qquad (2)$$

where $\psi_n(\mathbf{r})$ is the wavefunction of the bound electron and $\varphi_\varepsilon(\mathbf{r})$ is the wavefunction of the positron. To obtain accurate results, we need to ensure convergence of correlation corrections (e.g., Fig. 1 (b)) with respect to the maximal angular momentum of the electron and positron intermediate states included in the calculation. In our calculations, we calcuated the spectra $w(\epsilon)^{[l_{\max}]}$ for values up to $l_{\max} = 8$ and extrapolated the result according to [3],

$$w(\epsilon) = w(\epsilon)^{[l_{\max}]} + \frac{C}{l_{\max} + 1/2}, \qquad (3)$$

where C is a constant.

In Fig. 2 the spectra obtained by using the 0th and 1st-order diagrams [4], (a) and (b) in Fig. 1, are compared with experimental data [1, 5].

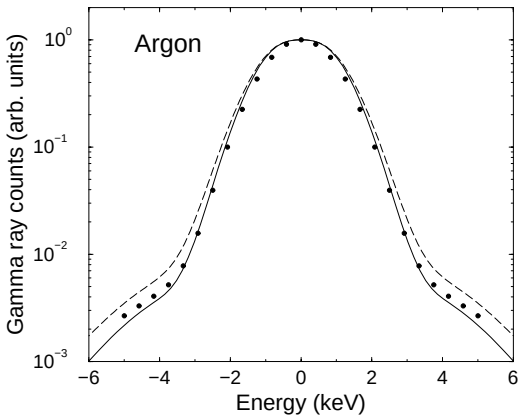


Fig. 3. Annihilation spectra for Ar normalised to unity at $\epsilon = 0$: dashed curve, 0th-order diagram, Fig. 1 (a); solid curve, 0th and 1st-order diagrams, Fig. 1 (a), (b); solid circles, experiment [1, 5].

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POSITRONIUM FORMATION FROM VALENCE AND INNER SHELLS IN NOBLE GASES

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Recently, positronium (Ps) formation in positron collisions with noble gas atoms has been determined by two experimental groups [1, 2]. The two sets of data are in fairly good agreement. However, when compared to recent theoretical results the agreement is qualitative but not quantitative [3]. In previous theoretical works only Ps formation with valence and subvalence electrons had been studied. We want to re-examine it and study Ps formation with the inner-shell electrons. The latter process can contribute to the production of inner-shell vacancies in positron-annihilation-induced Auger spectroscopy, a tool used to detect impurities on surfaces [4].

The 1st-order amplitude of the formation of Ps($1s$) by a positron of energy ε and an electron from the atomic orbital n is $\langle\tilde{\Psi}_{1s,\mathbf{K}}|V|n\varepsilon\rangle$, where V is the electron-positron Coulomb interaction and $\tilde{\Psi}_{1s,\mathbf{K}}$ is the wavefunction of the ground-state Ps atom with momentum $\mathbf{K}$, $\Psi_{1s,\mathbf{K}} = e^{i\mathbf{K}\cdot(\mathbf{r}+\mathbf{r}')/2}\varphi_{1s}(\mathbf{r}-\mathbf{r}')$. The tilde above $\Psi_{1s,\mathbf{K}}$ indicates that this wavefunction is orthogonalised to the electron orbitals n' occupied in the atomic ground state [5],

$$|\tilde{\Psi}_{1s,\mathbf{K}}\rangle = \Big(1 - \sum_{n'} |n'\rangle\langle n'|\Big)|\Psi_{1s,\mathbf{K}}\rangle \qquad (1)$$

The cross section proportional to $\left|\langle\tilde{\Psi}_{1s,\mathbf{K}}|V|n\varepsilon\rangle\right|^2$, is found by expansion in the positron partial waves (up to $l = 10$).

Figure 1 shows the Ps formation cross sections by the $3p$ and $3s$ electrons in argon and compares them with the experimental data. Our theoretical values (similiar to those of [3]) overestimate the experimental results, especially at low energies. We believe that this is primarily due to the limitation of the Born approximation for the low-l partial waves, e.g., the p- and d-wave contributions at positron momenta $k \approx 1$ au are at or above the unitarity limit, $\pi(2l+1)/k^2$.

Figure 2 shows Ps formation from all subshells in Ar. Around 500 eV the cross-sections are similar in magnitude and the inner-subshell contribution takes over at higher energies.

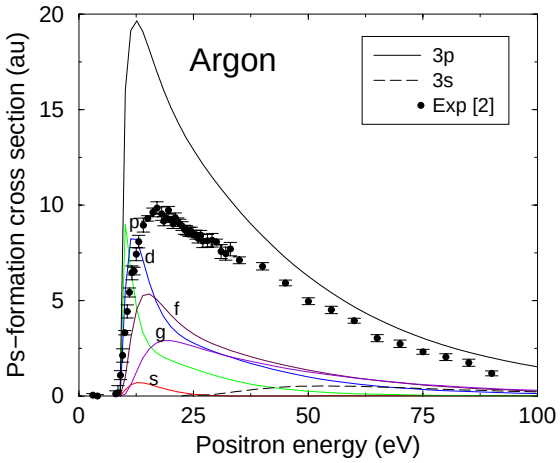

Fig. 1. Low-energy Ps formation in Ar, with partial wave contributions shown for the $3p$ subshell.

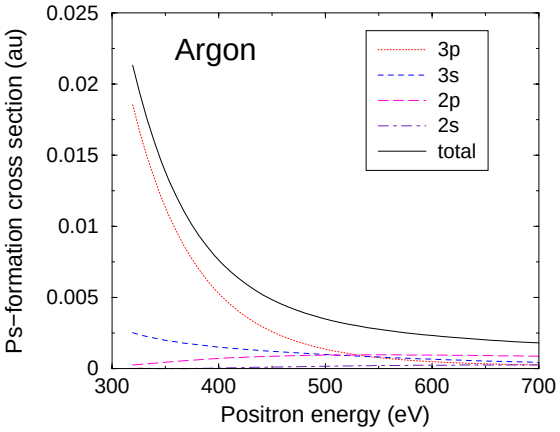

Fig. 2. Ps formation at higher energies.

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Faddeev three-body approach to high-energy positronium formation

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Three-body interaction is of interest in many areas of physics and technology. Faddeev, Watson and Lovelace (referred to as the FWL method [1]) developed one of the most successful fully quantum mechanical three-body theories which is particularly applicable at moderate and high scattering energies. Alston [2], Alt et al [3] and Ghanbari Adivi et al [4] applied the method to electron transfer in the collision of simple and complex atoms by ionic projectiles. A double scattering mechanism suggested by Thomas for forward electron transfer at high impact velocities, classically, is evident in all of these approaches. The existence of such a process has to show a peak, Thomas peak, about the Thomas angle, $\theta_T \cong \sqrt{3}\, m/M_P$, relative to forward direction, where m and M_P are the electron and projectile masses, respectively. The angular distributions are different in shape and relative magnitude around the critical angle 0.47 *mrad*. The methods used and developed are especially applicable at small angles.

Positronium is formed in the collision of poitrons with atomic species. This is also a three body interaction [5]. The Faddeev-Watson-Lovelace (FWL) scattering formalism is generalized to large scattering angles by applying to the positronium formation in the collision of positron with the atomic hydrogen at high impact energies as a three-body problem. In a second-order approximation, the integral forms of the five nuclear-electronic and inter-nuclear partial amplitudes are derived. The Coulomb two-body off-shell transition matrices are used to evaluate the closed forms of the amplitudes. Differential cross sections for positronium formation based on the quantum-mechanical FWL theory in the positron-hydrogen collisions are presented to confirm the presence of the Thomas peak. The results are shown in figure 1 for positron energies of 1.0 keV to 3.0 keV. As it is expected, the Thomas peak appears at about 60° angle which is the evidence of a double mechanism.

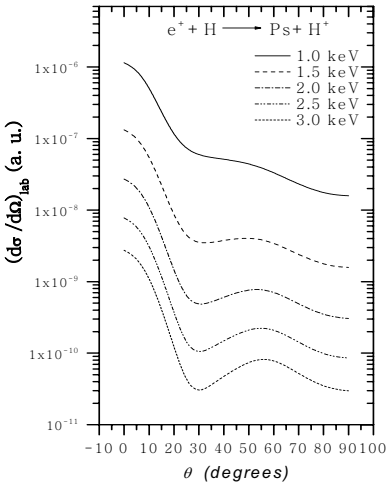

Figure 1. Differential cross sections calculated for the positronium formation in the collision of positron with atomic hydrogen.

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THRESHOLD POSITRON SPECTROMETER FOR STUDYING ATOMS AND MOLECULES

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Threshold positron impact studies, which distinguish and detect positrons scattered by atoms and molecules, could be very important, because the selection rules are much more relaxed when compared with those applied for example to photoionization processes and also to electron scattering experiments. Various important processes occur in threshold positron impact excitation of atoms and molecules, by instance, resonance formation, positronium formation, annihilation, as well as energy exchange due to post-collision interactions. In the present work we present a threshold positron impact spectrometer, which is being developed for studying positron collisions with atoms and molecules in the energy range up to 150 eV. The spectrometer consists essentially of an electrostatic positron beam, an effusive gas source and a positron analyzer based on the penetrating field technique [1,2] for the efficient collection of threshold (nearly zero energy) positrons. The analyzer can be tuned to accept threshold positrons (< 20 meV) and work with a power resolution better than 700, with a high signal/noise ratio. The electrostatic positron beam uses a ^{22}Na source and a tungsten wire array moderator as "monoenergetic" positron generator. These low energy positrons are extracted, focalized and collimated at the entrance of an 127^{o} electrostatic deflector using electrostatic lenses. Positrons selected by the deflector are accelerated and focalized at the collision region by another electrostatic lenses system.

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REARRANGEMENT CROSS-SECTION FOR HYDROGEN-ANTIHYDROGEN SCATTERING

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Observations of the first antimatter atom, the antihydrogen ($\overline{H}$) has created a renewed interest in the investigation of matter-antimatter systems. Recently cold $\overline{H}$ atom has been obtained in large numbers by the experimentalists at CERN [1]. Theoretical studies have been performed to understand the mechanism that permits trapping and cooling of antihydrogen ($\overline{H}$). The knowledge of the rates of elastic and inelastic atom-antiatom collision is of key importance. The elastic cross section is responsible for cooling and the inelastic one, particularly the rearrangement cross section ($H+\overline{H} = Ps + Pn$), is the measure of the loss of antihydrogen via annihilation.

The H-$\overline{H}$ collision system has been investigated by different groups [2-5]. Froelich *et al* [2] and Jonshell *et al* [3] have investigated the problem in the framework of Born-Oppenheimer (B-O) separation model. They have predicted s wave elastic and cross section. Armour and his coworkers [4] have investigated H-$\overline{H}$ scattering using Kohn variational principle in the framework of B-O separation. They have also predicted s-wave elastic and rearrangement cross-section. Results of rearrangement cross-sections obtained by theses two groups differ from each other. Both the groups have employed adiabatic model to investigate the problem in the Kelvin region. Ghosh and his collaborators [5] have investigated the problem using close coupling model. Their model is *ab initio* and non adiabatic in nature. Their elastic results are found to be reliable.

Here we investigate H-$\overline{H}$ collision system with the inclusion of rearrangement channel using close coupling model. In the calculation Ps atom is held fixed in the ground state and three protonium excited atomic states (22s to 24s) are retained. In the direct channel we have employed an elaborate basis sets. Convergence of results has been found. We report the results of direct and rearrangement cross-section and scattering length up to the incident energy 10^{-2} a.u. in the conference.

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POSITRON IMPACT IONIZATION OF CO, CO_2 AND CH_4

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Positron impact phenomena are theoretically simpler than the electron impact phenomena because of the lack of electron exchange and are considered a good testing ground for different theoretical models. Lately there has been a lot of research dealing with positron ionization phenomena. Until very recently all this work related to total (integrated) cross sections.

The theoretical calculations of these cross sections concentrated on the use of distorted wave models. Our group produced a number of theoretical papers [1,2] which showed that these models can, with various degrees of accuracy, reproduce the experimental measurements.

More recently our work concentrated on positron impact ionization of molecules. We found that for homonuclear molecular targets such as H_2, N_2, O_2 our distorted wave model CPE produces cross sections which agree well with the experimental results [3-5]. CPE is a relatively simple model in the sense that it does not require elaborate descriptions of the various scattering channels. Our calculations used a two-center approach with a Gaussian representation of the molecules.

In this work we applied the same approach to the positron impact ionization of CO, CO_2 and CH_4 for which experimental data is available [6]. Fig.1 shows that our theory is in excellent agreement with the experimental CO data. For CO_2 and CH_4 our theory produces cross sections significantly higher than the experiment results and we examine methods to improve this agreement.

Our work demonstrates that our relatively simple distorted-wave model can produce good results for heterogeneous molecular targets too.

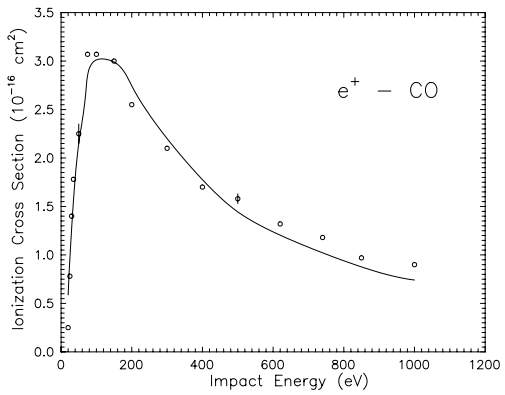

Figure 1. Positron impact ionization of CO: open circles correspond to the experiment of ref.[6], while the continuous curve corresponds to our CPE model.

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ORTHO-POSITRONIUM — ORTHO-POSITRONIUM SCATTERING AT LOW AND MEDIUM ENERGIES

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The interactions of many positrons and many positroniums are of topical interest for their application in different branches of Physics. Till date very few theoretical *ab initio* calculations on the scattering of positronium (Ps) atoms [1-4] have been carried out and all of them are restricted to s-wave only. The reason for this is the difficulty to evaluate exchange matrix elements, which are multidimensional and multicentered.

The motivation of the present article is to study o-Ps—o-Ps scattering and give estimate of elastic as well as inelastic cross sections at low and medium energies. We have employed plane wave model in which effect of exchange is included by antisymmetrizing the total wave function of the system. We report the integrated cross sections for (i) excitation of one of the Ps atoms (single excitation) (ii) simultaneous excitation of both the Ps atoms (double excitation) for n=2 and n=3. In addition to this we also report single and double ionization of Ps atoms. We have also performed the partial wave calculations for elastic and excitation processes. We notice a peculiar behaviour of partial wave cross sections. Only even values of partial wave survive for even parity transitions and vice versa. To the best of our knowledge this feature has not been noticed for other systems.

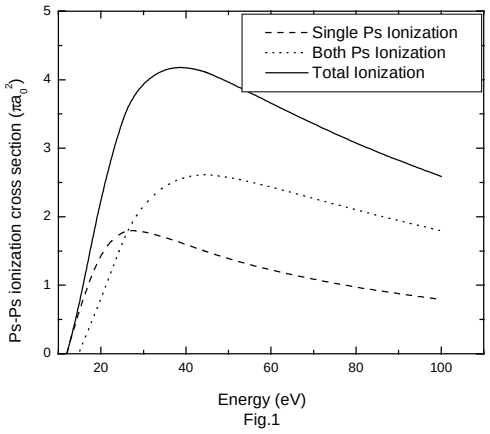

Fig.1

In fig. 1 we present single, double and total ionization cross sections from the threshold to 100 eV. It has been found that major contribution to the total cross sections arises from the double ionization processes. Detailed results will be submitted at the conference.

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PHOTON-PLASMON TRANSITION 2^3S_1-1^3S_1 IN THE POSITRONIUM: S-MATRIX FORMALISM CALCULATION

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It is well known that the positronium Ps is an exotic hydrogen isotope with the atomic mass $M=2m_e\sim1$ milli-amu and ground state binding energy of E=6,8 eV. The hfs states of Ps differ in spin S, life time t and mode of annihilation: para-Ps (S=0; $t=1{,}25\cdot10^{-10}n^3$ s ; 2γ annihilation) and ortho-Ps (S=1,$t=1.4\cdot10^{-7}n^3$ s ; 3γ annihilation). As a rule, probabilities of the cascade radiation transitions are more than the annihilation probability. The ortho-Ps atom has a metastable state 2^3s_1 and probability of two-photon radiation transition from this state into 1^3s_1 state ($1.8\cdot10^{-3}$ s^{-1}) is significantly less than probability of the three-photon annihilation directly from 2^3s_1 level ($8.9\cdot10^5$ s^{-1}), i.e. it is usually supposed that the ortho-Ps annihilates from 2^3s_1 state. Another situation may take place in plasma, where it is arisen the competition process of destruction of the metastable level – the photon-plasmon transition 2^3s_1-1^3s_1 with emission of photon and Langmuir quanta. In this paper we develop a new approach to calculation of the probability of the photon-plasmon transition in the Ps. In the theory of radiative and nonradiative decay of the quasistationary states of multielectron atom it is well known an energy approach (c.f. [1,2]), based on the adiabatic Gell-Mann and Law formula for the energy shift with electrodynamic scattering matrice. The method is a consistently electrodynamic one, allowing for the uniform consideration of a variety of induced & spontaneous processes. Earlier it has been with great success used in calculation of the radiation transition probabilities and oscillator strengths for different atomic and ionic systems [1-4]. The approach represents the decay probability as an imaginary part of energy shift dE, which is defined by S-scattering matrix of second (and higher) orders. Standard S-matrix calculation with using an expression for tensor of dielectric permeability of the isotropic plasma and dispersion relationships for transverse and Langmuir waves [3] allows getting the corresponding probability P(ph-pl). Numerical value of P(ph-pl) is $5.2\cdot10^6\cdot U_L$ (s^{-1}), where U_L is a density of the Langmuir waves energy. Our value is correlated with estimate, available in literature [3]: P(ph-pl)=$6\cdot10^6\cdot U_L$ (s^{-1}). Comparison of the obtained probability with the life time t(3γ) allows getting the condition of predominance of the photon-plasmon transition over three-photon annihilation. It is very important that considered transition may control the population of 2^3s_1 level and search of the long-lived Ps state can be used for diagnostics of the plasma turbulence.

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A complex-rotation calculation for resonances in Ps^- embedded in Debye plasmas*

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With the recent developments in laser plasmas produced by laser fusion in laboratories [1], and the continued interest of atomic abundances in astrophysics plasmas, as well as the recent activities on cold plasmas, it is important to have accurate atomic data available in the literature for atoms in various plasma environments. In the Debye-Hückel model for plasmas, the interaction potential between two charge particles is represented by a Yukawa-type potential, $\phi(r_a, r_b) = Z_a Z_b \exp(-|r_a - r_b| / \lambda_D) / |\vec{r}_a - \vec{r}_b|$, where $\mathbf{r_a}$ and $\mathbf{r_b}$ represent respectively the spatial coordinates of particles A and B, and Z_a and Z_b denote their charges. The parameter λ_D, called the Debye screening length, is a function of temperature and number density of the charge particles in the plasma. The smaller values of λ_D are associated with stronger screening. Using the stabilization method, we have recently made a first investigation on the $2s^2\ ^1S^e$ autoionization resonance in Ps^- embedded in various model plasma environments [2]. Here, we employ an alternate approach, a complex-rotation method [3], to study higher-lying resonances in Ps^-. The non-relativistic Hamiltonian (in Rydbergs) describing the negative positronium ion in Debye plasmas is

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{2}\nabla_3^2 - \frac{\exp(-r_{13}/\lambda_D)}{r_{13}} - \frac{\exp(-r_{23}/\lambda_D)}{r_{23}} + \frac{\exp(-r_{12}/\lambda_D)}{r_{12}},$$

where 1, 2, and 3 denote the two electron 1, 2 and the positron respective and r_{ij} is the relative distance between the particle i and j. For S-states we use Hylleraas-type wave functions to describe the system,

$$\Psi_{kmn} = \sum_{kmn} C_{kmn} (\exp[-\alpha(r_{13} + r_{23})] r_{12}^k r_{13}^m r_{23}^n + (1 \leftrightarrow 2)) \ ,$$

with $k + m + n \le \omega$, and ω, l, m and n are positive integers or zero. In the present work, wave functions with up to ω=18 (N=715) are used. In the complex-rotation method, the radial coordinates are transformed by $r \to r\, e^{i\Theta}$, and the kinetic and potential parts of the Hamiltonian are transformed to the form of $-(1/2)\nabla^2 e^{-2i\Theta}$ and $-(1/r)$¢í^{i}Ð¢ñ$\Theta}$ $\exp(-re^{i\Theta}/\lambda_D)$, respectively. Fig.1 and Fig.2. show, respectively, the resonance energy and width for the $3s^2\ ^1S^e$ resonance state as a function of $1/\lambda_D$. More results will be reported at the meeting.

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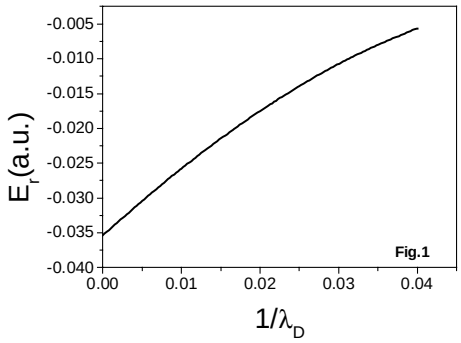

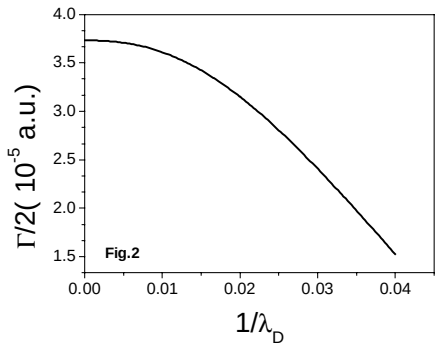

POSITRON SWARMS IN ARGON

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Recently systematic measurements have been made of positron atom cross sections and it has become possible to compile complete sets of cross sections and to calculate parameters for positron swarms. In this paper we have tried to compile such a set for argon, and to compare the calculated transport coefficients to those of electrons in the same gas.

Total cross sections were measured by Kauppila and coworkers [1] and total elastic cross sections were calculated by McEchran [2]. The two sets agree fairly well but we have selected the theoretical data as the basis because it allowed us to separate elastic and inelastic processes. We have extrapolated the theoretical results to low and high energies, and to obtain the summed (total) cross section we have added the inelastic cross sections. The positronium formation and ionization were taken from Marler et al [3] while direct annihilation has been neglected. Measured excitation cross sections for the lowest states of argon were used [4]. We have also added the cross section for higher singlet levels for electron excitation [5] of argon. As the energy dependence of both the elastic and inelastic cross sections for electrons and positrons is completely different, we may expect all aspects of positron transport to differ significantly from that of electrons. Positronium formation will lead to the loss of positrons and therefore will be analogous to electron attachment in electron transport. At the same time, ionization will not lead to an increase of the number of positrons so it should be treated as an inelastic, conservative process.

We have performed calculations by using a new Monte Carlo program that has been tested to give good benchmark results for electrons, especially in treatment of non-conservative transport [6]. The results show the effect of positronium formation which sweeps the distribution function below the threshold until E/N becomes sufficiently high.

E/N (Td)	mean energy (eV)	V_{dr} (flux) m/s	V_{dr} (bulk) m/s	D_T/μ (flux) (V)
1	3.55	5780	2271	2.88
5	3.97	27160	458	3.27
10	4.12	52710	266	3.28
50	5.00	21650	5700	4.08
100	5.88	36190	27830	4.56
500	13.40	913900	342100	7.22

Table 1 Transport coefficients for positrons in argon

At the same time, transport coefficients (shown in Table 1) show a huge effect of non-conservative collisions due to positronium formation, as the bulk drift velocity becomes almost two orders of magnitude smaller than the flux drift velocity. At higher E/N, however, the two drift velocities have the same order of magnitude. An interesting feature of these results is the relatively slow increase of the mean energy and of D_T/μ while the drift velocity increases by several orders of magnitude.

The transport coefficients were calculated for swarms of positrons in pure argon. Their basic features follow the standard effects of non-conservative transport, in this case due to positronium formation. Positron transport for a model gas was discussed by Robson [7] and our results are in general agreement with his predictions.

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Calculation of Z_{eff} using the SMC method with an optical potential

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The annihilation of positrons with molecules has been a source of major studies in the past years. The high annihilation rates encountered in the experimental data are still puzzling. Many models have been proposed to explain the phenomenon, but up to date none have given a completely satisfactory explanation [1].

The Schwinger Multichannel Method was originally created to calculate the low energy electron scattering by molecules [2], being later adapted for positron scattering and for the calculation of the annihilation parameter (Z_{eff}) [3]. The success obtained for the differential (DCS) and integral cross section (ICS) was not followed on the calculation of Z_{eff} [4]. This can be explained by two major reasons: the SMC method is a variational method for the scattering amplitude (and therefore for the calculation of the ICS and DCS), but not for the Z_{eff} parameter. The other reason is that it uses Cartesians Gaussians as basis set on the expansions of the bound and continuum molecular orbitals. These are smooth functions and do not reproduce the "cusp" always present in virtual positronium states.

In an attempt to better understand the high values found for the Z_{eff}, an optical potential initially proposed by Ivanov and Mitroy and later applied by Igarashi *et al.* [5] was included in the SMC method in order to make the calculation of the annihilation parameter variationally stable. In this work, the potential will be described and the first results obtained for the Helium atom and the Hydrogen molecule will be shown [6]. A basis set study for the He atom will be presented as a way to obtain the functions that could better reproduce the behavior encountered in the calculation of the Z_{eff}.

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COULOMB-BORN-OPPENHEIMER APPROXIMATION IN Ps-Atom SCATTERING

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A direct approach of evaluating the nine-dimensional exchange amplitude for ionization of positronium (Ps) in Ps-Atom scattering is developed using a Coulomb-Born-Oppenheimer approximation (CBOA). The present methodology is extremely useful to evaluate ionization cross section for different target systems and for different types of ionization processes. It is applied to calculate the Ps-ionization cross section and to estimate the effect of exchange in Ps-H [1] and Ps-He [2,3] systems. A continuum Coulomb wavefunction is used for the ionized electron to consider the effect of continuum instead of using a few selected discrete pseudostates as in coupled-channel R-matrix theory [4,5]. The results are compared with available experimental data of Ps-ionization in Ps-He [6] system.

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RESONANCES IN Ps-H SCATTERING

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A sudden change in phase shift by π radian is known as resonance. If it is in the s-wave and below inelastic threshold then it indicates a binding in the system. An accurate calculation is required for successful identification of a resonance. A complete and exact calculation is performed for collision of positronium (Ps) by hydrogen (H) using the best 3-channel projectile-inelastic [1] close-coupling approximation (CCA) for both the singlet and triplet channels. Resonances are observed in s-wave elastic phase shifts in both the channels below the inelastic threshold. The resonance in singlet channel is in agreement with the earlier prediction [2-5]. The resonance in triplet channel indicates a new type of binding. Detailed is being presented at the conference.

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