Collisions and spectral line shapes

The scientific cooperation between the laboratory DAMAP, now LERMA (Paris Observatory, CNRS UMR 8112, France) and Milan S. Dimitrijević, AOB, from 1978 to the present

Sylvie Sahal-Bréchot

Observatoire de Paris, LERMA CNRS UMR 8112, France

Subject: "Stark" broadening and shifting of spectral "isolated" lines of neutral and ionized atoms in the "impact" approximation

Calculations using the semiclassical-perturbation theory(1969, thesis, A&A), and Fortran "SCP" code of S.Sahal-Bréchot, updated and exploited.

Results: More than 150 publications and the STARK-B database















The birth of the cooperation: 1978

Exchange of letters with

P. Grujić, H. Van Regemorter, and S. Sahal-Bréchot

Beograd, 20.04. 1978

INSTITUT ZA FIZIKU
BEOGRAD
Studentski trg 16/III
Poštanski fah 57
P. Grujić

Dear Henri

As you probably remember, we planned to send postgraduate Mr Milan Dimitrijević to Paris, and you agreed that he might spend some time at your Laboratory at Meudon. Unfortunately, he did not get a grant for that last year, but recently he was aworded by a three months scholarship. We wonder if your agreement is still valid and whether he could spend two or three months at Meudon, working with some people there. We have primarily in mind Dr S. Sahal-Brechot, since it is yours and hers work that Mr Dimitrijević knows the best.

Dr. P. GRUJIC

Dr. P. GRUJIC

INSTITUT ZA FIZIKU BEOGRAD

Studentski trg 16/III

Postanski fah 57

Bear Dr. GRUJIC,

I have been charged by Henri VAN REGEMORTER to reply to your two letters of April 20th, 1978 concerning the stay of Mr. Milan DIMITRIJEVIC in our laboratory for two or three months at the next autumn.

We think this will be possible and we accept your proposition with pleasure. I have discussed with Henry and Nicole FEAUTRIER the various subjects of work that Mr. DIMITRIJEVIC could study during his stay. We arrived at the conclusion that he could work with Nicole FEAUTRIER and myself on the subject of the broadening and shift of Li 2s 2p perturbed by electrons.

Infact it should be very interesting to do a detailed comparison between

the close-coupling quantum approach and the semi classical perturbation approximation, in order to understend where quantum effects take place and where the semi classical approach fails down. The calculations should be made at rather high temperatures (10⁴ - 2 &6⁴) where the semi classical approach gives good results and at low temperatures (5 10 3K or less) where quantumseffects are expected. As a matter of fact, the Institute of Physic

of BEOGRAD (PURIC et al., J. Phys. B 10, 2375, 1977) recent measurements have been made on this line of Li at high T (1.5 104 at higher) but not at

low T.

NSTITUT ZA FIZIKU
BEOGRAD
Sudenski rg. 16/III
Poltzaki fah 57
P. Grujić

Dear Dr Sahal-Brechot

I am writing to you with regard to our postgraduate Mr Milan Dimitrijević, who would like to spend some time in your Laboratory, working on some problems in the Theory of Stark Broadening. We wonder if you would be willing to accept Mr Dimitrijević as a collaborator, since it is yours and Henri's work he is acquainted the best with. Last year Henri agreed to accept Mr Dimitrijević at Meudon and I have written a letter to him for his reaproval for his stay for two or three months there.

P. Grujić
INSTITUT DE PHYSIQUE
INSTITUTE OF PHUSICS
Beegraf - Yegoslatia
Sosiemski trg 16/III
P. O. Bex 57

Dear Dr. Sahal-Brechot
Many thanks for your letter of June 9th, concerning
the proposed stay of Mr. M. Dimitrijević at your Laboratory.

Many thanks for your letter of June 9th, concerning the proposed stay of Mr. M. Dimitrijević at your Laboratory. We are very glad your group is willing to accept him to stay three months there and colaborate with Dr. N. Feautrier and yourself.

The subject you have suggested seems quite interesting to us, both from theoretical and experimental point of view.



The beginning of the cooperation: the end of the seventies

2 visits of Milan to our laboratory:
Paris Observatory, DAMAP, CNRS GR24
And first paper in J.Phys.B: 1981, 14, 2559-2568
The first one of a long series!

Comparison between quantum and semiclassical calculations of the electron impact broadening of the Li I resonance line

M S Dimitrijevic[†], N Feautrier and S Sahal-Bréchot Observatoire de Paris, 92190 Meudon, France



The eighties: development of the cooperation

- International context: great expansion of Stark broadening researches, theoretical and experimental
- Needs for many theoretical results for comparison with experiments, and vice-versa
- Growing of the interest in astrophysics for many spectral lines and many elements, neutral and ionized, and for regularities.
- I gave all my computer codes to Milan.
- He coupled them to the Bates and Damgaard method for obtaining an atomic structure subroutine, coupled to many levels taken from the existing literature. He introduced in the code a test for verifying that the line studied is isolated.
- This permitted to obtain many results of Stark spectral lines widths and shifts for various temperatures and various electron and ion densities.

The two founding papers: JQSRT, 31, 301-313, 1984 and A&A, 136, 289-298, 1984

J. Quant. Spectrosc. Radiat. Transfer Vol. 31, No. 4, pp. 301-313, 1984 Printed in Great Britain.

0022-4073/84 \$3.00 + .00 © 1984 Pergamon Press Ltd.

STARK BROADENING OF NEUTRAL HELIUM LINES

M. S. DIMITRIJEVIC† and S. SAHAL-BRÉCHOT Observatoire de Paris, 92190 Meudon, France

(Received 25 March 1983)

Abstract—Using a semiclassical approach for the Stark broadening of atomic lines, we have calculated electron and proton impact line widths and shifts of 56 neutral He lines in the ultraviolet, visible and i.r. region of the spectrum. The comprehensive set of results obtained is used for investigation of Stark-broadening parameter regularities within the spectral series.

Density: 10¹⁶ cm⁻³

T= 10⁴ to 2 10⁵ K, and 5000 to 80000 K

Astron. Astrophys. 136, 289-298 (1984)



Stark broadening of neutral helium lines of astrophysical interest. Regularities within spectral series

M. S. Dimitrijević* and S. Sahal-Bréchot

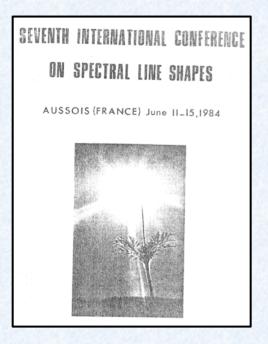
Observatoire de Paris, F-92190 Meudon, France

Received September 30, 1983; accepted February 8, 1984

Density: 10^{13} cm⁻³, $4 \le n \le 10$, T= 10^4 to $2 \cdot 10^5$ K, and 5000 to 80000 K.



1984: first ICSLS participation



Spectral Line Shapes

François Rostas, Sylvie Gordon (Eds.)

PROCEEDINGS SEVENTH INTERNATIONAL CONFERENCE AUSSOIS, FRANCE, JUNE 11-15, 1984 STARK BROADENING OF He I LINES OF ASTROPHYSICAL INTEREST : REGULARITIES WITHIN SPECTRAL SERIES AND INFLUENCE OF DEBYE SHIELDING

M.S. Dimitrijevic and S. Sahal-Bréchot Observatoire de Paris-Meudon 92125 Meudon Cédex, France

*Present address : Institute of Physics, P.O. Box 57 11001 Beograd, Yugoslavia

By using a semiclassical-perturbation formalism for the Stark broadening of atomic lines, we have calculated electron and proton impact linewidths and shifts of 36 neutral He I lines as the continuation of our previous work (1). These Stark broadening parameters have been calculated for lines originating from upper energy levels with 4 < n < 10, and for an electron density of $10^{13}~{\rm cm}^{-3}$, typical of stellar atmospheres.

Eighties: following years

 Scientific context on line broadening of spectral lines: many experiments, and continuation the development of the theories born in the sixties, study of regularities, systematic trends...

Several visits of Milan

(1 or 2 months per year to Meudon, supports from Paris Obs., exchange Agreements CNRS-French Foreign Ministry, Serbian Academy of Science and Arts...)

- Results for neutral and low-ionized atoms of astrophysical and experimental laboratory plasma research and industrial interest
- Study of regularities, behaviors as functions of T, N, n for obtaining new data and discussing the experimental results
- Several publications: Phys Rev A, JQSRT, AAS, BOAB: Na I, K I, Li I



End of the eighties and Nineties Scientific context:

 Considerable development of the study of stellar interiors, subphotospheric envelopes and stellar atmopheres:

Progresses in observations: ground-based telescopes and spaceborn missions.all domains of wavelengths from XUV to infrared

development of powerful computers stimulated the development of atomic data on a large scale; e.g. Phoenix code for stellar modeling

- Development of plasma research: laboratory, magnetic fusion, inertial confinement fusion, technological
- Needs of extensive sets of atomic data, Stark broadening among others. A great number of data needs a simple, fast and enough accurate method: ⇒ interest of the SCP code
- Birth of the interest for databases (IAU General Assembly 1994)



End of the eighties and Nineties

Several visits of Milan at the end of the eighties and in the beginning of the nineties, then pursuit of the cooperation through e-mail and Fax

- Extension of the data entries in the SCP code for obtaining results for several densities in a same run, with a check of the impact and isolated line approximations in the tables of results
- Extension of the code (Mg I) for infrared lines issued of high levels of neutral atoms, the colliding ions being neither H⁺ nor He⁺
- New effort for highly charged ions and lines originating from high levels, with an improvement of the codes (cooperation with V. Bommier for that).
- Exploitation of the code (especially Z>3): many publications)
- However: difficulties for publishing a great number of results, due to the lack of space: only paper existed at that time.
- Fortunately, ftp appeared in 1993 (or about), tables of results could be downloaded, only a few results appeared on the journal (paper)
- Developments of Internet, reviews on line, tables online



The new century: 2000-2010 years

 Growing of the interdisciplinary research between astrophysics and nuclear physics: formation of elements by nucleosynthesis, neutron capture for heavy elements (heavier than Fe)

⇒Importance of stellar measurements and needs of accurate spectroscopic diagnostics of weak lines (low abundances elements, often neutral).

Increasing development of the Virtual Observatories and databases

2003: Come back of Milan to Paris Obs. (Meudon)
Numerous visits to Paris Obs. (Meudon) followed

The new century: 2005-2015 years

The Virtual Observatory (International Virtual Observatory Alliance)

STARK-B (birth fall 2008) http://stark-b.obspm.fr

Need to exploit the huge amount of data produced by both ground and space based observational programmes

framework for organizing data bases and services:

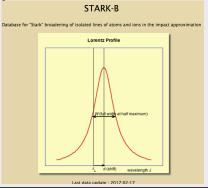
standardisation of data structures and access protocoles, interoperability

Paris Obs.:creation of Paris Data Centre/OV-Paris

LERMA: recruitment of **engineers** and **technicians** for databases

Recruitment of a research scientist: **Marie-Lise Dubernet**

- 2005: Scan of our "old" published data by a LERMA technician
- 2007-2008: first implementation (engineer Nicolas MOREAU) of the data.
- Fall 2008: STARK-B opened online, though very incomplete!
- Stark-B is a part of the databases of the Paris Observatory, with a link to SERVO
- End 2012: all our SCP data (more than 150 publications) implemented
- Since the end of 2013: implementation of the MSE data calculated by the AOB team.



VAMDC (2010-2013) VAMDC consortium (since 2013)

M L Dubernet et al.: J. Phys. B: At. Mol. Opt. Phys. 49 (2016) 074003

Virtual Atomic and Molecular Data Centre Consortium

http://www.vamdc.eu/ resp.M.L.Dubernet
http://www.vamdc.org/

- worldwide federation consortium
- interconnection of atomic and molecular databases
- e-science infrastructure
- organisation to support this activity.
- interpretation and modeling in astrophysics and plasmas.
- STARK-B is a part of the connected databases
 - http://portal.vamdc.org/vamdc_portal/nodes.seam
 - Resp.scientists: S.Sahal-Bréchot and M.S. Dimitrijević
 - Resp. technics and website: N. Moreau
 - Coop with N. Ben Nessib



The new century: since 2005 Cooperation Paris-Tunis-AOB

Merging of the cooperation Paris-Tunis (S. Sahal-Bréchot and N. Ben Nessib, after N. Ben Nessib thesis, 1995) **and of the cooperation AOB-Tunis** (M. Dimitrijević and N. Ben Nessib, since 1989).

 NBN coupled of the SCP code to TOPbase (R-matrix with innovative asymptotic techniques) by NBN.

Result: C II widths and shifts for white dwarfs (pub MNRAS with N. Larbi-Terzi)

The students of N. Ben Nessib joined our cooperation:

Besma Zmerli (thesis and SCP paper on Cu I, for technological application) **Neïla Larbi-Terzi** (CII pub)

Haykel Elabidi (quantum SST+DW impact Stark widths of ionized atoms, thesis and papers)

Walid Mahmoudi (SCP extension of the quadrupolar potential to very complex atoms, thesis and papers)

Rafik Hamdi coupled the SCP code to the Cowan's atomic structure code (interest for complex atoms) thesis and papers.

They used also with Milan the Modified Semiempirical Method(MSE) for some complex atoms

NBN for STARK-B: fitting formulae as functions of T (2011)



The future

- Pursuit of calculations of line widths and shifts for needs in modeling and spectroscopic diagnostics, and Implementation in STARK-B
- Implementation of our quantum results
- Creation of other fitting formulae (regularities, systematic trends) for STARK-B
- Improvement of the calculation of the shift
- The SCP code on line?
- And, after us, I hope that the new generation will continue, modernize and update the methods and the codes...
 - Andjelka Kovacević, Zoran Simić, Nenad Milovanović, Haykel Elabidi, Rafik Hamdi, Walid Mahmoudi, Magdalena Christova..., and students, present and to come...

Happy Birthday, Milan! Thank you for this so fruitful cooperation, and Many returns of the day!

And acknowledgements to the official agencies who support this cooperation









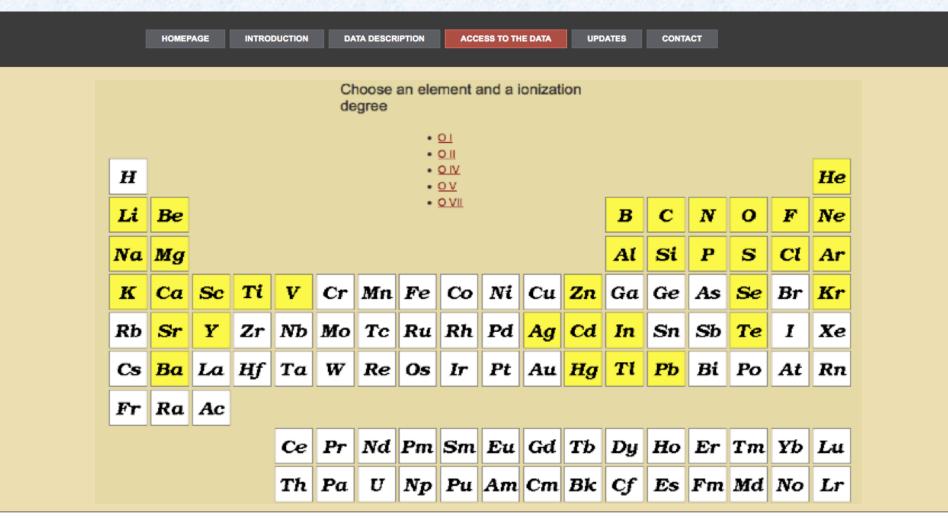


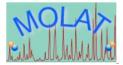


Thank you for your attention

Additional slides (if questions or comments)

STARK-B: Access to the data (2008)

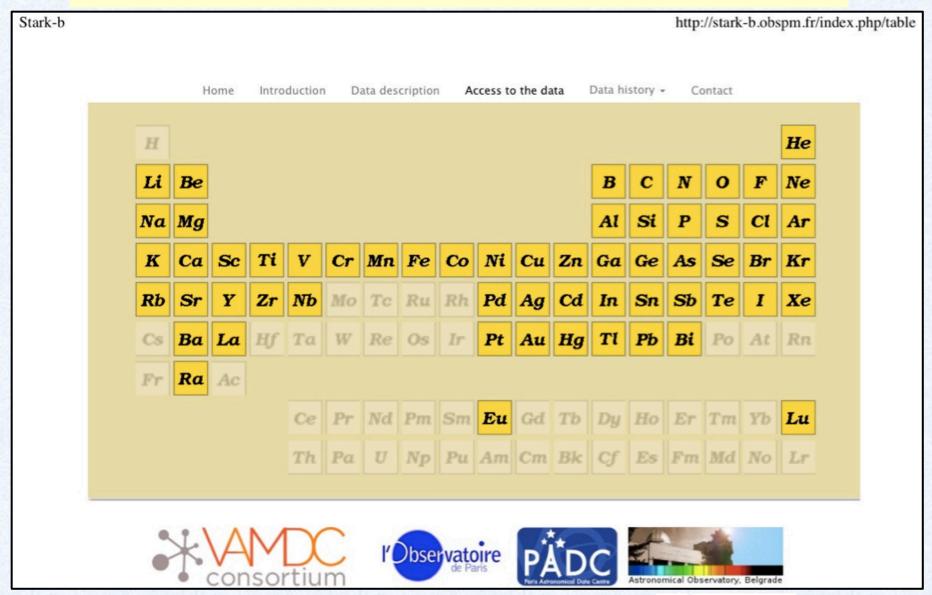








STARK-B: Access to the data (2017)



Autumn 2008 - Autumn 2013: **SCP** published data **inserted** for 123 neutral and ionized atoms

(more than 150 publications)

current stage: insertion of new or updated data as son as they are published

	Ag I,	Mg I, Mg II, Mg XI
	Al I, Al III, Al XI	Mn II
	Ar I, Ar II, Ar III, Ar VIII	N I, N II, N III, N IV, N V
	Au I	Na I, Na X
	B II, B III	Ne I, Ne II, Ne III, Ne IV, Ne V, Ne VIII
	Ba I, Ba II	Ni II
	Be I, Be II, Be III	O I, O II, O III , O IV, O V, O VI; O VII
	Br I	P IV, P V
	C II, C III, C IV, C V	Pb IV
	Ca I, Ca II, Ca V, Ca IX, Ca X	Pd I
	Cd I, Cd II	Rb I
	CI I, CI VII	S III, S IV, S V, S VI
	Cr I, Cr II, Cu I	Sc III, Sc X, Sc XI
	F I, F II, F III ,F IV, F V, F VI, F VII	Se I
	Fe II	Si I, Si II, Si IV, Si IV, Si V, Si VI, Si XI, Si XII, Si XIII
	Ga I	Sr I
	Ge I, Ge IV	Te I
	He I	Ti IV, Ti XII, Ti XIII
	Hg II	TI III
	H	V V, V XIII
	In II, In III	YIII
	K I, K VIII, K IX	Xe VI, Xe VIII
	Kr I, Kr II, Kr VIII	Zn I
	Li I, Li II	

Since end 2013:

Current stage: insertion of MSE data about 90 neutral and ionized atoms

(about 70 publications)

Ag II Al III, Al V Ar II, Ar III, Ar IV As II, As III Au II B III, B IV Ba II Be III Bi II, Bi III Br II C III, C IV, C V Ca II Cd II, Cd III CI III, CI IV, CI VI Co II, Co III

Cu III, Cu IV

Eu II, Eu III FIII, FV, FVI Fe II Ga II, Ga III Ge III, Ge IV \mathbf{H} Kr II, Kr III La II, La III Lu III Mg II, Mg III, Mg IV Mn II, Mn III N II, N III, N IV, N VI Na III, Na VI Nb III Nd II Ne III, Ne IV, Ne V, Ne VI, Ne VII, Ne VIII

O II, O III, O IV, O V PIII, PIV, PVI Pt II Ra II SII, SIII, SIV Sb II Sc II Se III Si II, Si III, Si IV, Si V, Si VI, Si XI Sn III Sr II, Sr III Ti II, Ti III VII, VIII, VIV Xe II $Y \parallel$ Zn II, Zn III Zr II, Zr III

Beograd, 20.04. 1978

INSTITUT ZA FIZIKU BEOGRAD Studentski trg 16/III Poštanski fah 57 P. Grujić

Dear Henri

As you probably remember, we planned to send post-graduate Mr Milan Dimitrijević to Paris, and you agreed that he might spend some time at your Laboratory at Meudon. Unfortunately, he did not get a grant for that last year, but recently he was aworded by a three months scholarship. We wonder if your agreement is still valid and whether he could spend two or three months at Meudon, working with some people there. We have primarily in mind Dr S. Sahal-Brechot, since it is yours and hers work that Mr Dimitrijević knows the best.

Mr Dimitrijević is completing his PhD thesis here, under the supervision by Dr N. Konjević and myself, and it is expected that he would have his oral examination by September this year. The title of the Thesis is: "The Influence of the Long-Range Potentials on the Stark Broadening of Spectral Lines from Plasmas". I am enclosing reprint of a recent paper by Mr Dimitrijević and myself, which contains a part of his Thesis.

Dr A. Lesage, who spent two weeks here recently, the best thing suggested that, regarding the accomodation, would be an early coming in September and renting a room somewhere at Meudon, since there is, presumably, two weeks limit for keeping a room at the very Laboratory.

A shall write a separate letter to Dr Sahal-Brechot.

How is your work going on? You must be very busy
with running the Laboratory. How are Lan, Maryivonne, David,
Dr Feutrier and Dr Tran Minh? Please remember me to them and to
your most kind secretary, too.

Best wishes,

Defer

P. Grujić

INSTITUT ZA FIZIKU BEOGRAD Studentski trg 16/III Poštanski fah 57 P. Grujić

Dear Dr Sahal-Brechot

I am writing to you with regard to our postgraduate Mr Milan Dimitrijević, who would like to spend some time in your Laboratory, working on some problems in the Theory of Stark Broadening. We wonder if you would be willing to accept Mr Dimitrijević as a collaborator, since it is yours and Henri's work he is acquainted the best with. Last year Henri agreed to accept Mr Dimitrijević at Meudon and I have written a letter to him for his reaproval for his stay for two or three months there.

Mr Dimitrijević is a very hardworking person, well acquainted with the physics of Stark broadening. He should finish his PhD thesis, under the title "The Influence of Long-Range Fotentials on the Stark Broadening of Spectral Lines from Plasmas", by September this year. I am enclosing a paper by Mr Dimitrijević and myself, which covers a part of his Thesis. Some other papers by Mr Dimitrijević are enclosed, too.

We would appreciate very much if you could accept Mr Dimitrijević to work with you, what would be very benefitial for his postdoctoral work.

Sincerely yours,

P. Grujić

78

Dr. P. GRUJIC INSTITUT ZA FIZIKU BEOGRAD Studentski trg 16/III Postanski fah 57 BEOGRAD

Dear Dr. GRUJIC,

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We think this will be possible and we accept your proposition with pleasure. I have discussed with Henry and Nicole FEAUTRIER the various subjects of work that Mr. DIMITRIJEVIC could study during his stay. We arrived at the conclusion that he could work with Nicole FEAUTRIER and myself on the subject of the broadening and shift of Li 2s 2p perturbed by electrons.

Infaatt it should be very interesting to do a detailed comparison between the close-coupling quantum approach and the semi classical perturbation approximation, in order to understand where quantum effects take place and where the semi classical approach fails down. The calculations should be made at rather high temperatures ($10^4 - 2~\&6^4$) where the semi classical approach gives good results and at low temperatures (5 10 3 K or less) where quantumseffects are expected. As a matter of fact, the Institute of Physics of BEOGRAD (PURIC et al., J. Phys. B 10, 2375, 1977) recent measurements have been made on this line of Li at high T (1.5 10^4 at higher) but not at low T.

Do you think that your colleagues might make a second experiment at lower T ?

Since Mr. Milan DIMITRIJEVIC has already studied short range effects in line broadening (your paper of JQRST, 1978) we hope that this sort of subject will interest him.

Concerning the accommodation I agree with the suggestion of Dr. A. LESAGE. I propose that we should exchange other mails in order to settle practical details relative to his exact date of arrival in France and our possibilities of housing at the MEUDON Observatory.

Expecting to hear from you soon, I remain,

Sincerely yours?

Sylvie SAHAL-BRECHOT

Dear Dr. Sahal-Brechot

Many thanks for your letter of June 9th, concerning the proposed stay of Mr. M. Dimitrijević at your Laboratory. We are very glad your group is willing to accept him to stay three months there and colaborate with Dr. N. Feautrier and yourself.

The subject you have suggested seems quite interesting to us, both from theoretical and experimental point of view. Mr. Dimitrijević had word with Dr. J. Purić, who told him that an experiment at lower temperatures $(T \le 10^3)^{0}$ K) would be feasible in their laboratory and that they could carry out the measurements proposed.

As for the accomodation at Meudon, we hope that it won't be the problem, though Mr. Dimitrijević will probably have to postpone his arrival there for month or so. Completition of his PhD thesis is, namely, in delay, partly because of family reasons, so that he will be able to submit his Thesis somewhen in September. We shall inform you in time, anyway, about a possible exact date of his arrival.

Plese convey my best regards to Henri and my thanks for the preprint by Tran Minh at al., I received the other day. Remember me to Drs. Feautrier, Tran Minh, LeDourneuf and VoKyLan, too.

Best wishes.

P. Guyi

Petar Grujić

Dr. S. SAHAL-BRECHOT
Observatoire de Paris
Section d'Astrophysique
92190 MEUDON
F r a n c e

Comparison between quantum and semiclassical calculations of the electron impact broadening of the Li I resonance line

M S Dimitrijevic†, N Feautrier and S Sahal-Bréchot Observatoire de Paris, 92190 Meudon, France

Received 23 December 1980, in final form 2 March 1981

Abstract. We present quantum mechanical calculations of Stark broadening parameters for the Li 12s 2S-2p 2P line. Semiclassical calculations have also been performed and both have been compared with other available results. A detailed analysis of Stark broadening parameters as functions of the impact electron angular momentum quantum number and of the temperature is carried out. The influence of the polarisation potential and of the completeness of the set of energy levels on the Stark broadening parameters is investigated. The low temperature behaviour of the half width is discussed too.

1. Introduction

In spite of the existence of very successful semiclassical treatments (e.g. Sahal-Bréchot 1969a, b, Griem 1974) for electron collisional broadening parameters, it is interesting to perform sophisticated quantum mechanical calculations. Our purpose is in fact to provide a quantitative check of the different approximations which are made in the usual semiclassical perturbation treatments. We have chosen the case of a neutral atom. As a matter of fact, whereas the dominant angular momentum of the colliding electron varies between 3 and 15 for ion emitters because of the long range of the Coulomb field, for neutrals it lies typically between 1 and 5 (Bely et al 1963). Therefore, short-range effects are more important and this will facilitate the discussion concerning this important aspect of the semiclassical treatment (cut off and strong-collisions terms). Moreover, the effect of the exchange should be more important for neutrals and this is typically a quantum process. We have chosen the resonance line of Li 1 (2s 2S-2p 2P) because the polarisability of Li is very large both in the fundamental and excited states and therefore the importance of the polarisation potential, which is also a short-range effect, will be easier to discuss.