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Theoretical Transition Probabilities and Lifetimes

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Abstract

The beam-foil method and the computation of oscillator strengths with correlated wave functions both had their beginning in the late 1960s. The stimulating interplay between theory and experiment will be reviewed. With the power of todays computers, great progress has been made in computation. The current state of spectrum calculations using the multiconfiguration Hartree-Fock method will be described and the importance of relativistic effects mentioned.

1. Introduction

Atomic spectra and energy levels of B I – V were still incompletely known in 1970. In a paper published by Martinson, Bickel, and Ölme [1] at that time, 17 new lines were classified, the wavelengths of 29 new lines measured with some suggested transitions, and 38 lifetimes reported. The method used was the newly developed beam-foil method [2] whose use proliferated during the 1970's providing extensive data for both neutral and highly ionized atoms. This data was of great benefit to theory.

Even though boron has relatively few electrons, theoretical calculations were limited and those for B I and B II were considered to be only 50% accurate. Thus the boron paper contained no comparison with theory, only with other experimental methods.

The 1960's was a period in which theory was developing the use of stored program electronic computers and their application to atomic structure properties. The FORTRAN compiler was formally released in 1957 but did not become widely available until the early 1960's. Until that time, programs were written in either machine or assembly code specific to the widely varying hardware of the computers. With the availability of the FORTRAN compiler, programs became portable and for the first time it was feasible to develop code that could be used with modest effort on different computers. Memory was still a severe constraint and the first multiconfiguration Hartree-Fock (MCHF) program published in 1969 [3] was dimensioned for interaction matrices of at most 5×5. The emphasis was also very much on "understanding the physics." With larger matrices the ability to visualize the interaction was impaired to the extent that some scientist considered such calculations "numerology." Today it is recognized that for accuracy from an *ab initio* configuration interaction model, exceedingly large matrices will be needed.

The late 1960s and the 1970's were devoted largely to learning about the effect of correlation on the oscillator strength and its behavior along an iso-electronic sequence. An excellent example is the $3s^23p\ {}^2P^o - 3s3p^2$ and $3s^23d\ {}^2D$ transitions [4]. Because these two configuration states (CSFs) interact strongly, the two ^2D states, which we shall refer to as ^2D_u and $^2D_\ell$ for upper and lower respectively, have wave functions that exhibit considerable mixing. In fact, the dominant configuration state of $^2D_\ell$ changes from $3s^23d$ for the nuclear charge $Z = 13$ to $3s3p^2$ for higher Z. But, when plotting the transition matrix element, it is the matrix element for the lower and upper that are continuous functions of Z, as shown in Figure 1. The short curves are Hartree-Fock results. The length and velocity results for $^2D_\ell$ are in excellent agreement but the transition energies are wrong, demonstrating clearly that agreement of the two gauges is a necessary but not sufficient condition. The figure also shows that the effect of configuration interaction on the transition matrix element for the upper state is one of enhancement whereas the effect on the lower state is cancellation. In fact, the latter transition matrix element changes sign along the sequence. It is also seen that the effect of the interaction remains significant over a wide range of nuclear charges. Such interactions are considered "long range" interactions whereas some, often in regions of a cross-over, are "short range". Transition calculations in those days were "hand-crafted" with considerable trial and error in the inclusion of configuration states in the wave function. In 1975, Nicolaides and Beck [5] proposed a first-order theory for oscillator strengths (FOTOS) which identified the configuration states that contributed to the matrix elements to first order. The transition energy was not considered.

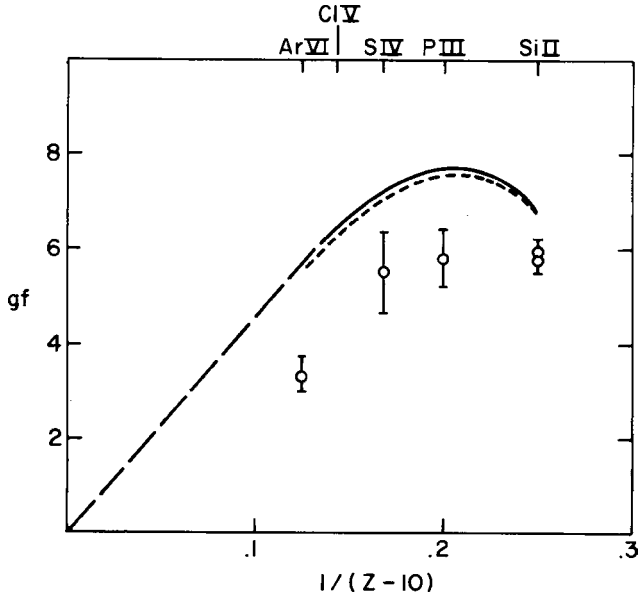

Fig. 1. The effect of correlation on the transition matrix element.

Beam-foil methods were providing a wealth of data for iso-electronic sequences, making possible a mutually beneficial comparison between theory and experiment. When cancellation occurs, the matrix element is more likely to be in error, thus it was a

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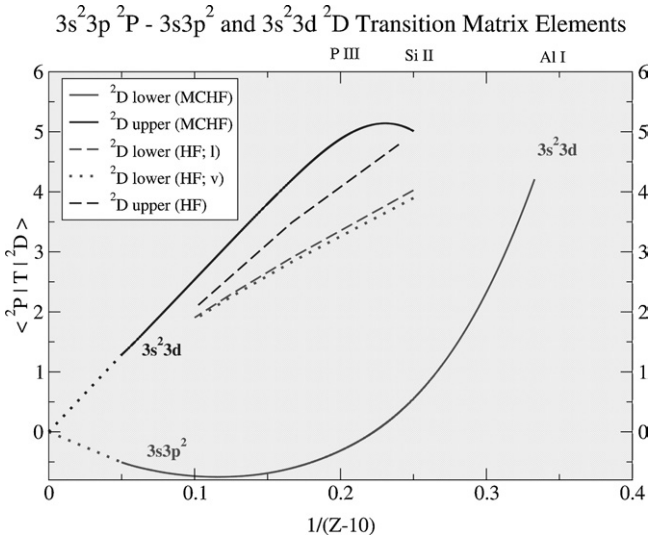

Fig. 2. The weighted oscillator strength for the $3s^2 3p\ ^2P^o - 3s^2 3d\ ^2D_u$ transition.

surprise in 1976 to learn that the oscillator strengths for transitions to $^2D_\ell$ were in better agreement with beam-foil data than for ^2D_u where there was enhancement [6, 7]. Figure 2 shows a typical trend. The experimental values for Si II are from Ref. [8, 9] and the others from Ref. [10].

Martinson *et al.* [11] analyzed a number of sequences of interest in fusion research. Good agreement with calculations that included correlation was usually found though the values tended to diverge from each other as Z increased. Cascading was known to be a problem and simulated decay curves were produced that showed cascading to become less serious as Z increased. In a paper on the discrepancies between theoretical and experimental oscillator strengths of the sodium sequence [12], extensive computer simulated decay curves were produced and the conclusion was that the 3p meanlife should be extractable. The later computer simulation by Younger and Wiese [13] went a bit further and showed clearly that the customary multi-exponential fitting methods could not accurately extract the lifetime of the 4p level in the similar copper sequence. In 1985, a renewed study of singly ionized boron was published by Bashkin *et al.* [14]. By this time, there was extensive comparison with numerous theories and agreement was excellent, often differing by less than 5%. But the lifetime of $2s3s\ ^1S_0$ was missing.

2. Systematic methods

Early calculations were guided by theories such as FOTOS [5] or Z-dependent theories for oscillator strengths [6]. Such theories neglected the fact that it was necessary to predict both the transition energy *and* the transition matrix element accurately. The multiconfiguration Hartree-Fock (MCHF) achieved this through the introduction of systematic methods [15] for both energies and matrix elements.

The non-relativistic multiconfiguration Hartree-Fock (MCHF) approach is used for calculating the wave function Ψ for the state labeled γLS,

$$\Psi(\gamma LS) = \sum_i c_i \Phi(\gamma_i LS), \tag{1}$$

where γ usually represents the dominant configuration, and any additional quantum numbers required for uniquely specifying the state. The MCHF wave function Ψ is expanded in terms of configuration state functions (CSFs) (Φ) having the same LS symmetry but arising from different electronic configurations or couplings (γ_i). The CSF's are built from a basis of one-electron spin-orbital functions

$$\phi_{nlm_l m_s} = \frac{1}{r} P_{nl}(r) Y_{lm_l}(\theta, \varphi) \chi_{m_s}. \tag{2}$$

The MCHF procedure [16] consists of optimizing to self-consistency *both* the sets of radial functions $\{P_{n_i l_i}(r)\}$ and mixing coefficients $\{c_i\}$. Thus the CSFs included in the expansion determine the radial functions.

In large scale methods, systematic calculations are performed of increasing size that allow the monitoring of properties under investigation. In such systematic methods, active sets (AS) of orbitals are used to determine the expansion. These are characterized by the largest principal quantum number. Thus the $n = 3$ active set consists of all the orbitals $\{1s, 2s, 2p, 3s, 3p, 3d\}$, though it should be remembered that for correlation orbitals (orbitals not occupied in the Hartree-Fock approximation), the principal quantum number is not important spectroscopically, but serves as a simple index for the orbital of a given symmetry. Given an active orbital set, rules are used to generate the CSF expansion according to some model. Generally there is an inactive core that does not participate in the correlation. The remaining electrons may include some filled shells and open or valence shells. It is essential to include valence correlation and configurations that account for the polarization of filled shells by the valence electrons, also referred to as core-valence correlation. For high accuracy, it may be important to include correlation in the filled shells.

The rules for obtaining expansions are often expressed in terms of a number of excitations – singles (S), doubles (D), etc. However, in order to allow for the degeneracy of orbitals at higher Z, it is convenient to express the rule in terms of the set of possible principal quantum numbers. To curb the rate of growth of the expansions with the orbital set size, it may be convenient to define the CSF set as the union of two sets. Typically, systematic methods perform a series of calculations where the rules are applied to active sets of increasing size.

Through the use of systematic methods, and the biorthogonal transformation to compute transition matrix elements between two wave functions whose orbitals have been optimized independently [17], a very accurate line strength was obtained for the resonance transition of sodium which, when corrected for a small relativistic effect, was in near perfect agreement with the most recent experimental analysis, resolving a long standing discrepancy between theory and experiment [18]. It also is possible to monitor convergence of the transition energy and the length and velocity forms of the line strength as a check on the correlation model. If the transition energies converge, but length and velocity line strengths are not in adequate agreement, some significant correlation has been neglected by the model.

Table I shows some typical examples from B II. For the $2s2p\ ^1P^o - 2s3s\ ^1S$ transition, the transition energies have converged, the velocity form of the line strength is quite stable, but the length value is still decreasing. This is an example where the velocity form is the more stable, but note the cancellation in the line strength of almost two orders of magnitude in going from $n = 3$ to $n = 10$. For the $2s^2\ ^1S^o - 2s3p\ ^1P$ transition, the transition energies have converged to a fraction of a cm^{-1} and the two values of the line strength agree to four significant digits.

Table I. *LS trends for some transitions in B II.*

n	$\Delta E(\mathrm{cm}^{-1})$	S_l	S_v
$2s2p\ ^1P^o - 2s3s\ ^1S$			
3	64323.23	0.19487E+00	0.12393E+00
4	64430.35	0.56963E−01	0.17070E−01
5	64289.21	0.17475E−01	0.54420E−02
6	64251.51	0.67517E−02	0.32807E−02
7	64251.83	0.42708E−02	0.26336E−02
8	64257.85	0.34656E−02	0.24064E−02
9	64259.85	0.28858E−02	0.22607E−02
10	64260.02	0.26510E−02	0.22252E−02
$2s^2\ ^1S^o - 2s3p\ ^1P$			
4	144348.64	2.37153D−01	2.47256D−01
5	144179.85	2.45036D−01	2.46718D−01
6	144162.67	2.46939D−01	2.48330D−01
7	144147.52	2.47682D−01	2.48190D−01
8	144145.61	2.48183D−01	2.48370D−01
9	144145.39	2.48394D−01	2.48433D−01
10	144145.15	2.48499D−01	2.48517D−01

Table II. *Theoretical spectrum for B II up to* $2s3d\ ^1D_2$.

Config.	LS	J	Energy (cm^{-1})	Splitting	τ (s)
$2s^2$	$^1S^o$	0	0.00		
2s2p	$^3P^o$	0	37468.95		
		1	37475.16	6.20	9.529e−02
		2	37491.43	22.47	5.792e+02
2s2p	$^1P^o$	1	73583.67		8.295e−10
$2p^2$	^3P	0	99236.79		1.146e−09
		1	99245.38	8.59	1.146e−09
		2	99258.85	22.06	1.146e−09
$2p^2$	^1D	2	102702.89		1.817e−08
$2p^2$	^1S	0	127993.86		7.471e−10
2s3s	^3S	1	129913.75		9.138e−10
2s3s	^1S	0	137859.05		6.309e−07
2s3p	$^3P^o$	0	144149.50		2.504e−08
		1	144150.73	1.23	7e−08
		2	144154.17	4.67	2.502e−08
2s3p	$^1P^o$	1	144278.16		1.688e−09
2s3d	^3D	1	150837.05		4.077e−10
		2	150837.16	0.11	4.077e−10
		3	150837.72	0.67	4.078e−10
2s3d	^1D	2	154881.70		7.214e−10

3. Spectrum calculations

Most recently, transition probability calculations have advanced from the study of individual lines to the study of the spectra of an isoelectronic sequence. This latter now requires that relativistic effects be included. That means that the configuration states in LS expansions for various terms must be concatenated and eigenstates of the interaction matrix for the Breit-Pauli interaction matrix determined. The MCHF method was extended so that orbital sets could be optimized for a weighted average of energy expressions for different LS terms or different eigenstates of an LS term [19]. Once orbitals sets for interacting LS terms were determined, the intermediate coupling LSJ wave functions for all levels of the terms could be determined from Breit-Pauli interaction matrices. Spectrum calculations used this scheme to compute all levels of a spectrum up to a certain level. From these wavefunctions, all possible E1 and some E2 and M1 transitions were computed from which the lifetimes of the levels could be determined. Table II shows the energy levels, their splitting relative to the lowest level of a term, and the lifetimes of levels in B II. Note that the lifetime of $2s3s\ ^1S$ is almost three orders longer than the lifetime of $2s3s\ ^3S$ which explains why it was so elusive in beam-foil experiments [20].

Such calculations produce extensive transition data for which an online web-based database was implemented together with a search capability facilitating the search of data in spectra or iso-electronic sequences [21]. Along with the theoretical data, the NIST energy level data [22] was included so that a search can yield some indication of accuracy. Table III shows part of this data. In addition to transition data, the error in the transition energy in percent, $E(\%)$, is provided along with the discrepancy in the transition probabilities between the two gauges in percent, $T(\%)$, for the 2s2p – 2s3s transitions. For the $^3P^o - {}^3S$ transition both accuracy indicators are high. One would expect similar accuracy for the $^1P^o - {}^1S$ allowed transition, but now the error in the transition energy has reached 3.23%. Fortunately, Martinson *et al.* have performed another beam-foil experiment with higher resolution and sensitivity and the $2s3s\ ^1S$ excitation energy has been revised [20]. Once the NIST energies are revised, the error in the singlet-singlet transition energy reduces to 0.10% but because of the cancellation seen in Table I, the discrepancy

Table III. *Results of a database search for* 2s2p – 2s3s *transitions. Included are the theoretical wavelengths λ, the line strength S, the transition probability A_{ki}, the error in the transition energy E(%) and the difference in the transition probabilities in length and velocity T(%).*

g_i	g_k	λ	S	f_{ik}	A_{ki}	$E(\%)$	$T(\%)$
$^3P^o - {}^3S$							
1	3	1081.73	2.278e−01	6.397e−02	1.216e+08	0.01	0.7
3	3	1081.80	6.837e−01	6.399e−02	3.647e+08	0.01	0.7
5	3	1081.99	1.140e+00	6.403e−02	6.080e+08	0.01	0.7
$^3P^o - {}^3S$							
3	1	996.18	4.035e−08	4.101e−09	8.270e+01	2.12	4.9
$^1P^o - {}^3S$							
3	3	1775.26	2.917e−07	1.663e−08	3.521e+01	−0.08	−21.6
$^1P^o - {}^1S$							
3	1	1555.81	2.946e−03	1.917e−04	1.585e+06	3.23	13.0

$T(\%)$ is much larger than for the triplet-triplet transition. The error in the transition energy for the triplet-singlet transition reduces to 0.01%. Though with this correction to the observed energy excitation data, the transition energies are accurate to 0.1%, the discrepancy in the two gauges is larger. This can be attributed to cancellation in the case of singlet-singlet matrix elements but it also has to be recognized that the velocity form has omitted some relativistic corrections that may be more important in spin-changing transitions. Thus the length value that is used for determining the transition probability may be more accurate than the discrepancy might suggest.

Spectrum calculations have been computed for Be-like to Ne-like sequences [23] and Na-like to Ar-like are in progress.

4. Forbidden transitions

All examples so far have been for E1 transitions, but the forbidden E2 and M1 transitions are important in astrophysical studies and in night sky spectra. The decay of the $2p^3\ ^2D^o_{3/2,5/2}$ levels to the ground state has been observed in experimental data from

Table IV. *Transition probabilities for decay from* $2p^3\ {}^2D^o_{5/2,3/2}$ *levels of Nitrogen compared with observation.*

J	A_{ki} (E2)	A_{ki} (M1)	A (Total)	$A(J=5/2)/A(J=3/2)$
MCHF: 1984 [25]				
5/2	5.158	0.912	6.07	
3/2	3.365	14.84	18.21	0.333
MCHF: 2003 [23]				
5/2	6.595	0.971	7.566	
3/2	4.341	15.951	20.292	0.373
Experiment: 2003 [24]				0.370

Night Sky spectra obtained using the Keck I High Resolution Spectrograph [24]. This decay, via a combination of E2 and M1 transitions, had been computed by Godefroid and Froese Fischer [25] in 1984 with some concern that some relativistic corrections to the length form of the transition operator might be important in the case of this half-filled shell system. Table IV shows that the present, more highly correlated wave functions provide ratios of total decay rates, $A_{ki}(\mathrm{E2}) + A_{ki}(\mathrm{M1})$, that are in excellent agreement with intensities observed in night sky spectra. Thus any neglected relativistic terms are not of significance in this case.

Table V. *A detailed comparison of* $3p^6\ {}^1S_0 - 3p^5 4s\ {}^{1,3}P^o_1$ *with recent theory and experiment.*

	Energies			g_J	
Method	$^3P^o_1$	$^1P^o_1$	diff	$^3P^o_1$	$^1P^o_1$
Obs. [22]	93751	95400	1649	1.404	1.102
BP (present)	93346	94963	1617	1.416	1.085
MCDHF a)	92811	94407	1596	1.400	1.101
MCDHF b)	93438	95089	1606	1.402	1.098
RCI [27]	94526	96238	1712		
CI + RMBPT [29]	92595	95307	1712		

	f-values		
Source	$^3P^o_1$	$^1P^o_1$	Ratio
Experiment			
Federman *et al.* [30]	0.064	0.257	4.01
Chan *et al.* [34]	0.0662(33)	0.265 (13)	4.00
Ligtenberg *et al.* [26]	0.0616(21)	0.2297 (93)	3.73
Wu *et al.* [32]	0.0676(40)	0.2590 (150)	3.83
Gibson & Risley [33]	0.0580(17)	0.2214 (68)	3.82
Theory			
BP (fine tuned)	0.0619	0.2662	4.30
MCDHF a)	0.0570	0.221	3.87
MCDHF b)	0.0562	0.226	4.02
RCI [27]	0.0627	0.248	3.69
CI + RMBPT [29]	0.0629	0.254	4.03

5. Multiconfiguration Dirac-Hartree-Fock methods

For the light elements discussed here, the Breit-Pauli approximation is adequate but for heavy atoms or highly ionized systems, the multi-configuration Dirac-Hartree-Fock (MCDHF) theory is preferable. The calculations are more demanding but with increases in computer speed, may become quite feasible. Surprisingly, a recent study of Ar I has suggested that even for this neutral atom, MCDHF may be preferable.

The resonance transitions, $3s^3 3p^6\ {}^1S_0 - 3p^5 4s\ {}^{1,3}P^o_1$ have a long history going back as far as 1958. (An extensive list of references to experimental and theoretical data can be found in Ref. [26] and Ref. [27]). In table V, we analyze recent theoretical values and experimental data for these transitions more closely. In addition to f-values, we look also at the ratio of the f-values for the allowed and spin-forbidden transitions. It appears that experiment can determine this ratio more accurately than the f-values themselves. For the upper levels, we also compare with observed g_J factors which depend largely on the term composition of a level. Spectrum calculations for Ar I have been performed in the Breit-Pauli approximation where expansions were obtained by SD excitations from a multi-reference set [28]. For intercombination lines, there are a number of accuracy indicators. In addition to the excitation energy, there is the energy separation between the $^1P^o_1$ and $^3P^o_1$ levels which determines the extent of the mixing. It was $1617\,\mathrm{cm}^{-1}$ in our *ab initio* Breit-Pauli calculation and adjusted to $1638\,\mathrm{cm}^{-1}$ when diagonal term energy corrections were applied. Another is the spread of the $^3P^o$ multiplet which was $1305.40\,\mathrm{cm}^{-1}$ (not affected by adjusting) compared to $1413.91\,\mathrm{cm}^{-1}$ for the observed. This suggests that the relativistic effect was not large enough, and that the mixing of the $^1P^o_1$ and $^3P^o_1$ terms was too small. This is confirmed by the g_J factor that is too large for $^3P_1$ and too small for $^1P_1$. We therefore undertook also an MCDHF calculation for these transitions. Expansions were obtained through SD excitations $3s^2 3p^6$ and $3s^2 3p^5 4s$ for odd and even states, respectively, for $n = 3, 4, 5$. For the odd levels, calculation a) proceeded with the same scheme also for $n = 6$, but b) added core-polarization that emphasizes the outer region of the wave function important in transition calculations. The results are reported in table V and compared with experiment, first for energies and then for f-values. The Breit-Pauli (BP) energy is for the *ab initio* energy. Comparing with MCDHF, the Relativistic Configuration Interaction (RCI) performed by Avgoustoglou and Beck [27], and the most recent Configuration Interaction and Relativistic Many-Body Perturbation Theory (CI + RMBPT) by Savukov [29], the MCDHF b) energies are the best with the present Breit-Pauli (BP) a close second but the the computed g_J for the latter are not in good agreement with observed.

In the study of f-values, Federman *et al.* [30] measured the f-value for the allowed transition but used semi-empirical methods for estimating the value for the intercombination line and noted that the ratio of allowed to forbidden was about 4.0. Since then, there have been several accurate experimental measurements, and though the absolute values for their f-values differ, the ratios are considerably more constant, generally in the range of 3.8–4.0.

If the Breit Pauli f-values are corrected also for the their spread (as suggested by Hibbert in a process referred to as "fine-tuning" [31]) we get the values in the table, with a ratio of 4.30. The MCDHF ratios are in close agreement with the experimentally determined one, whereas the RCI value is too low and the CI + RMBPT one is too high. In addition, the MCDHF f-values are also in close agreement with the experimental values of Gibson and Risley. The considerable difference in the present Breit-Pauli and MCDHF f-values for the allowed transition, suggests relativistic effects were not captured accurately by the Breit-Pauli approximation. But there still is significant difference with the other relativistic theories. Thus further study is needed.

The heaviest element for which transition probabilities have been calculated is Lr ($Z = 103$). The MCDHF calculation

confirmed that the ground state was [Rn]$5f^{14}7s^27p\ ^2P^o_{1/2}$ [35]. The transition to [Rn]$5f^{14}7s^26d\ ^2D^o_{3/2}$ required wave function expansions of more than 330,000 CSFs. Unlike light elements, where core correlation can usually be neglected, in Lr it was found to be of extreme importance, affecting the oscillator strength by a factor of two. In the homologous Lu ($Z = 71$), the ground state is [Xe]$4f^{15}7s^25d\ ^2D_{3/2}$ and the methods used reproduced the observed transitions energy to within 126 cm^{-1}. The effect of correlation in the core affected the oscillator strength by a factor of 3. There are many heavy elements where correlation is still an unexplored territory and this study suggests there is much more to be learned and experimental data will be extremely valuable.

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