QUANTUM THEORY OF DIELECTRONIC RECOMBINATION

by

Jacques Anne Roland DUBAU

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ABSTRACT

The dielectronic recombination rate formula of Bates and Dalgarno is justified by using an accurate resonance profile theory and the time dependant perturbation method developped by Davies and Seaton . The formula of Burgess for the autoionisation probability is generalised to the many channel problem and applied to the delicate case of He^+ .

The symmetry between photoionisation and dielectronic recombination is proved and a generalised $\mathcal{S}$ matrix containing the photon interaction is deduced .

The method of extrapolation, in the case of $He^+ + e^-$, is simplified compared to Bely's method and a resonance profile is given that generalised Seaton's formula to this case .

A new formula obtained for the dielectronic recombination rate satisfies the two unitary conditions corresponding to the collision theory and photo-emission theory .

The calculated results are compared to those of Burgess and Shore .

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CHAPTER I

Introduction

The importance of the dielectronic recombination of ions in Astrophysical plasmas was first recognised by Massey and Bates (1942) . Subsequently Bates and Dalgarno (1962) derived a formula for the dielectronic recombination rate which has been used until now for practical calculations .

For evaluationg the autoionisation probability required in this formula two different methods were used ;
The first approach was given by Burgess (1964) in which he extrapolated the excitation cross section of the ion through the excitation threshold . This method proved to be excellent for the high excited states where the dielectronic recombination appeared to be important .
A second approach was developped by Trefftz (1967) . The idea of Trefftz was to solve the collision interaction by a distorted wave approximation and then treat the configuration interaction and the photointeraction both as perturbation .

In 1969 , Davies and Seaton gave a more rigourous formulation than Bates and Dalgarno .They supposed the problem of collision had been already solved and considered the photon interaction as a time dependent perturbation .

Shore (1969) simplified Trefftz method . The zero-order collision solution were screened hydrogenic radial functions . At the first order he neglected the coupling between resonances with the justification that " If n is sufficiently large , the configuration mixing caused by the Coulomb interaction is less significant than the spin-orbit interaction of the unexcited electron .... The neglect of configuration mixing with the use of Jl coupling should not introduce serious errors " .

In our method we use integro-differential coupled equations for the collision since in the case of He^+ the distorted wave approximation is valid only for $l \geqslant 5$. Compared to the autoionisation probability of the low partial waves , the partial wave for $l \geqslant 5$ are very small and can be neglected in the computation of the dielectronic recombination quantities .

We extrapolate the reactance matrices through the excitation threshold (2s,2p) using a generalisation of Burgess' method . We also consider all the coupling between resonances (closed-closed interaction) .

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CHAPTER II

Initial electron-ion system and final atomic wave functions

In this chapter we define the wave functions of the system neglecting radiation field interaction. These wave functions correspond to the initial (ion-free electron) system and final (ion-bound electron) system. They satisfy the Schrödinger wave equation, the relativistic interaction being neglected.

By decomposing these wave functions using a partial wave analysis we simplify the problem and obtain in the place of the pratically unsolvable Schrödinger equation a set of coupled integro-differential equations

The normalisation of these wave functions, the scattering $\underset{\sim}{S}$ matrix and the reactance $\underset{\sim}{R}$ matrix are then briefly outlined.

2-1 Coupled integro-differential equations

The Schrödinger equation of the system of two electrons, $He^+ + e^-$, is

$$(H - E)\ \Psi(x_1 x_2) = 0 \tag{2.1}$$

It contains partial derivatives that makes it pratically unsolvable in this form.

However solutions can be obtained by separating the variables (Fourier method). The idea is to write the solutions as an infinite sum of a product of functions, that each contains only one variable. Each function satisfies a differential equation. In our problem these functions of the variable $x_1 = (r_1, \hat{r}_1, \sigma_1)$ are solutions to the He$^+$ problem for which we know the exact solutions. For the functions for $\hat{r}_2, \sigma_2$ we take eigen functions of the angular momenta (Normalised Spherical Harmonic and Normalised Spin Function) . The only unknown function corresponds to the colliding variable r_2 .

These can be summarised by the following formulae :

$$\left.\begin{aligned} \Psi(x_1 x_2) &= \sum_\gamma \psi_\gamma(x_1 x_2) \\ \psi_\gamma(x_1 x_2) &= \Phi_\gamma(x_1 \hat{r}_2 \sigma_2)\,\frac{F_\gamma(r_2)}{r_2} \end{aligned}\right\} \quad (2.2)$$

$\Phi_\gamma(x_1 \hat{r}_2 \sigma_2)$ includes the wave functions of the He$^+$ electron and the angular and spin functions of the colliding electron

$$\Phi_\gamma(x_1 \hat{r}_2 \sigma_2) = \frac{1}{r_1} P_{n\ell}(r_1)\, Y_{\ell m_\ell}(\hat{r}_1)\, \chi(m_s|\sigma_1)\, Y_{\ell' m_\ell'}(\hat{r}_2)\, \chi(m_s'|\sigma_2) \quad (2.3)$$

with

$$\left.\begin{aligned} &\int P_{n\ell}(r)\, P_{n'\ell}(r)\, dr = \delta_{nn'} \\ &\int Y^*_{\ell m_\ell}(\hat{r})\, Y_{\ell' m_\ell'}(\hat{r})\, d\hat{r} = \delta_{\ell\ell'}\,\delta_{m_\ell m_\ell'} \\ &\int \chi(m_s|\sigma)\, \chi(m_s'|\sigma)\, d\sigma = \delta_{m_s m_s'} \end{aligned}\right\} \quad (2.4)$$

where γ denotes the coupling representation

$$\gamma = (n \ell m_\ell m_s \, k_n \ell' m_{\ell'} m_{s'}) \qquad (2.5)$$

$(n \ell m_\ell m_s)$ are the quantum numbers of the He$^+$ target and $(k_n \ell' m_{\ell'} m_{s'})$ the quantum numbers of the colliding electron .

Due to the conservation of the angular momenta it is better to use the following representation :

$$\Gamma = (n \ell k_n \ell' S L M_S M_L) \qquad (2.6)$$

Then we shall define

$$\left.\begin{aligned} \Psi'(x_1, x_2) &= \sum_{\Gamma} \Psi_{\Gamma}(x_1, x_2) \\ \Psi_{\Gamma}(x_1, x_2) &= \Phi_{\Gamma}(x_1, \hat{r}_2 \sigma_2) \, \frac{F_{\Gamma}(r_2)}{r_2} \end{aligned}\right\} \qquad (2.7)$$

with

$$\Phi_{\Gamma}(x_1, \hat{r}_2 \sigma_2) = \sum_{\gamma} (\Gamma|\gamma) \, \phi_{\gamma}(x_1, \hat{r}_2 \sigma_2) \qquad (2.8)$$

where

$$(\Gamma|\gamma) = C^{\ell \ell' L}_{m_\ell m'_\ell M_L} \, C^{\frac{1}{2} \frac{1}{2} S}_{m_s m'_s M_S} \qquad (2.9)$$

$C^{\alpha \beta \gamma}_{a b c}$ being the vector coupling coefficient (Clebsch-Gordon)

The transformation matrix between the radial solutions $F_{\gamma}(r_2)$, $F_{\Gamma}(r_2)$ will be seen later when we shall have studied the asymptotic form of these solutions.

In order to satisfy the Pauli principle we shall antisymmetrise $\Psi'(x_1 x_2)$ (or $\Psi(x_1 x_2)$) . In collision problem we have not the difficulty arising when the two electrons are equivalent .

$$\Psi_A(x_1 x_2) = \frac{1}{\sqrt{2}} \left\{ \Psi'(x_1 x_2) - \Psi'(x_2 x_1) \right\} \qquad (2.10)$$

Introducing (2.10) in (2.1) and using the hypothesis that Φ_{Γ} (or ϕ_{γ}) are a complete basis we have in place of (2.1) the following infinite set of equations

$$(\Phi_{\Gamma'} \mid H - E \mid \Psi_A) = 0 \qquad (2.11)$$

This in turn gives the infinite set of coupled radial integro-differential equations

$$\left\{ \frac{d^2}{dr^2} - \frac{l'(l'+1)}{r^2} + \frac{2}{r} + k_n^2 \right\} F_{\Gamma'}(r) = \sum_{\Gamma} U_{\Gamma\Gamma'}(r) F_{\Gamma'}(r) \qquad (2.12)$$

where $U_{\Gamma\Gamma'}$ is an integro differential operator (see Percival and Seaton (1957)).

$$U_{\Gamma\Gamma'} = 0 \quad \text{if} \quad L \neq L' \quad \text{or} \quad S \neq S'$$

(conservation of the angular momenta)

$U_{\Gamma\Gamma'}$ is independant of M_L and M_S (Racah tensor)

If we take, in (2.3), $P_{nl}(r)$ real and for $Y_{lm_l}(\hat{r})$ the classical normalised spherical harmonic $U_{\Gamma\Gamma'}(r)$ becomes symmetric and real.

$$U_{\Gamma'\Gamma} = U_{\Gamma\Gamma'} \qquad (2.13)$$

In chapter IV we shall use only the asymptotic expression of U

$$U_{\Gamma\Gamma'}(r) \underset{r\to\infty}{\sim} \frac{\alpha_{\Gamma\Gamma'}}{r^2} \qquad (2.14)$$

The partial wave analysis conserves the energy :

$$E = E^+_{n\ell} + \frac{k_n^2}{2} = E^+_{n'\ell'} + \frac{k_{n'}^2}{2} \qquad (2.15)$$

where $E^+_{n\ell}$ is the eigen energy of the target He$^+$ electron (nl) in a.u. (atomic unit) . We can renormalise the He$^+$ target energie so that they are equal to zero for the ground state and are positive for the excited states : $E^+(1s) = 0$, $E^+(2s) = E^+(2p) = 1.5$ a.u.

In practical computations it is impossible to solve an infinite number of coupled radial equations . We shall reduce the He$^+$ states to "1s" "2s" and "2p" states (they are usually called terms) giving 3 or 4 equations, (2.12), corresponding to the 3 or 4 elements of the summation for $\psi'(x_1 x_2)$. As we shall see in 2-2 for each energy E will correspond 3 or 4 independant physical solutions.

Using Kohn variational principle and formula (2.10) but not (2.11) it is possible to obtain the coupled equations (2.12) for the former approximate expansion (see Burke and Seaton (1971)

2-2 Asymptotic expression for open channels

We suppose all the $k_n^2 > 0$ (it is said that all the channels are open). By choosing the former convention for $P_{n\ell}(r)$ and $Y_{\ell m_\ell}(\hat{r})$ we said that $U_{\Gamma\Gamma'}$ becomes real and symmetric. Then every coefficient in the coupled integro-differential equations (2.12)

are real

and we can deduce that it is possible to find the same number of independant real function that it would have been for independant complex functions. Also it is easy to prove that the maximum number of independant solutions is $2 \times n$.

For large r, the equations (2.12) tend to coulomb equations and we can develop asymptotically the solutions on the coulomb solutions (regular and irregular)

$$F_{\Gamma i} \underset{r \to \infty}{\sim} \frac{1}{\sqrt{k_n}} \left\{ a_{\Gamma i} \sin(x) + b_{\Gamma i} \cos(x) \right\} \qquad (2.16)$$

Γ corresponds to the equation, i to the solution .

$$x = k_n r - \frac{l\pi}{2} + \frac{1}{k_n} \ln(2kr) + \arg \Gamma\left(l+1-\frac{i}{k}\right) \qquad (2.17)$$

Now by taking the physical boundary condition

$$F_{\Gamma i}(0) = 0 \qquad (2.18)$$

we eliminate half of the independant solutions.

Let's write a basis set satifying (2.18) on the matrix form (n,n)

$$\underset{\sim}{F} = \begin{pmatrix} F_{\Gamma i} \end{pmatrix} \qquad (2.19)$$

we have

$$\underset{\sim}{F} \underset{r\to\infty}{\sim} \frac{1}{\sqrt{k}} \left\{ \sin(x)\, \underset{\sim}{A} + \cos(x)\, \underset{\sim}{B} \right\} \qquad (2.20)$$

The matrices having the symbol "$\sim$" under them are ordinary matrices, the other ones are diagonal matrices e.g $\frac{1}{\sqrt{k}}$, $\sin(x)$, $\cos(x)$.

2-3 R and S matrices

We can also choose a basis set having the following asymptotic behaviour :

$$\underset{\sim}{F}(\underset{\sim}{R}, r) \underset{r\to\infty}{\sim} \frac{1}{\sqrt{k}} \left\{ \sin(x) + \cos(x)\, \underset{\sim}{R} \right\} \qquad (2.21)$$

where

$$\underset{\sim}{R} = \underset{\sim}{B}\, \underset{\sim}{A}^{-1} \qquad (2.22)$$

$\underset{\sim}{R}$ is called the reactance matrix for it represents the departure from the coulombic problem ($\underset{\sim}{R}_{coulomb} = 0$).

Using the Green theorem it can be proved that $\underset{\sim}{R}$ is symmetric (and real) because $\underset{\sim}{U}$ is symmetric (and real), see for example Mott and Massey (1965).

Due to the particular asymptotic form (2.21) we can denote the indices of $\underset{\sim}{F}(R, r)$ by Γ and Γ', Γ' is called "the entrance channel" and Γ is called "the final channel" : $F_{\Gamma\Gamma'}(\underset{\sim}{R}, r)$.

Let's define another set of solutions but this time a complex one :

$$\underset{\sim}{F}\,(\underset{\sim}{S}\,,r) \sim \frac{1}{\sqrt{k}}\left\{ \exp(-ix) - \exp(ix)\,\underset{\sim}{S} \right\} \qquad (2.23)$$

where

$$\underset{\sim}{S} = (1 + i\underset{\sim}{R})(1 - i\underset{\sim}{R})^{-1} \qquad (2.24)$$

$\underset{\sim}{R}$ being real and symmetric $\underset{\sim}{S}$ is symmetric and unitary .

On a similar way we can define $F_{\gamma\gamma'}$ corresponding to the representation γ (2.5) . The relation between $S_{\gamma\gamma'}$ and $S_{\Gamma\Gamma'}$ is

$$S_{\gamma\gamma'} = \sum_{\Gamma\Gamma'} (\gamma\,|\,\Gamma)\; S_{\Gamma\Gamma'}\,(\Gamma'\,|\,\gamma')$$

If we consider a coulombic plane wave of electron on an ion in the state $(n\ell m_\ell m_s)$ it is possible, after a partial wave decomposition, to relate $S_{\gamma\gamma'}$ to the probability of transition during the collision . Therefore $\underset{\sim}{S}$ has been called the scattering matrix . The conservation of the electron flux is a consequence of the unitarity of $\underset{\sim}{S}$:

$$\underset{\sim}{S}^{+}\underset{\sim}{S} = \underset{\sim}{S}\,\underset{\sim}{S}^{+} = 1$$

$\underset{\sim}{S}^{+}$ is the transpose conjuguate of $\underset{\sim}{S}$.

The relation between $\underset{\sim}{S}$ and $\underset{\sim}{R}$ can also be written :

$$\underset{\sim}{S} = (1 - i\underset{\sim}{R})^{-1}(1 + i\underset{\sim}{R}) \qquad (2.25)$$

This formula is sometimes useful (see Chapter IV (4.37))

2-4 Asymptotic expansion when some channels are closed

When some channels are open and some are closed the energies of some terms $E_{n''\ell''}$ are greater than E and the corresponding channels have a negative energy $k^2_{\Gamma''} < 0$. The coulombic solutions are then either divergent $\left(\frac{2r}{\nu''}\right)^{-\nu''} e^{\frac{r}{\nu''}}$ or convergent $\left(\frac{2r}{\nu''}\right)^{\nu''} e^{-\frac{r}{\nu''}}$ where $k^2_{\Gamma''} = -\frac{1}{\nu''^2}$ $(\nu'' > 0)$.

The physical solution which corresponds to an open entrance channel Γ has final channels being either open Γ' or closed Γ'' but for the closed channels the asymptotic $F_{\Gamma''\Gamma}$ must be convergent . By doing a linear combination of the n solutions we can eliminate the divergent part and obtain n' convergent physical solutions (n' equals the number of open channels, n" is defined as n"=n-n') .

Their asymptotic form is :

$$\left.\begin{aligned} F_{\Gamma'\Gamma}(\underset{\sim}{\mathcal{R}}, r) &\sim \frac{1}{\sqrt{k_{\Gamma'}}}\left\{ \sin(x')\delta_{\Gamma'\Gamma} + \cos(x')\mathcal{R}_{\Gamma'\Gamma} \right\} \\ F_{\Gamma''\Gamma}(\underset{\sim}{\mathcal{R}}, r) &\sim \left(\frac{2r}{\nu''}\right)^{\nu''} e^{-\frac{r}{\nu''}} d_{\Gamma''\Gamma} \end{aligned}\right\} \quad (2.26)$$

$\underset{\sim}{\mathcal{R}}$ is a (n',n') matrix. With $d_{\Gamma''\Gamma}$ we can form a matrix $\underset{\sim}{d}$ (n",n') . $\underset{\sim}{\mathcal{R}}$ is symmetric (and real) therefore we obtain from it a $\underset{\sim}{\mathcal{S}}$ matrix symmetric and unitary :

$$\left.\begin{aligned} F_{\Gamma'\Gamma}(\underset{\sim}{\mathcal{S}}, r) &\sim \frac{1}{\sqrt{k_{\Gamma'}}}\left\{ e^{-ix'}\delta_{\Gamma'\Gamma} - e^{ix'}\mathcal{S}_{\Gamma'\Gamma} \right\} \\ F_{\Gamma''\Gamma}(\mathcal{S}, r) &\sim \left(\frac{2r}{\nu''}\right)^{\nu''} e^{-\frac{r}{\nu''}} c_{\Gamma''\Gamma} \end{aligned}\right\} \quad (2.27)$$

where

$$\underset{\sim}{\mathcal{S}} = (1 + i\mathcal{R})(1 - i\mathcal{R})^{-1} \tag{2.28}$$

the relation between the $\underset{\sim}{C}$ matrix (n",n) and the matrix $\underset{\sim}{d}$ is

$$\underset{\sim}{C} = \frac{2}{i}\,\underset{\sim}{d}\,(1 - i\mathcal{R})^{-1} \tag{2.29}$$

($\underset{\sim}{d}$ is a real matrix)

2-5 Asymptotic expansion for all closed channels

When all the channels are closed it is no more a problem of collision but of bound states .

It is always possible to find for any negative energy E a basis set having the following asymptotic form :

$$\underset{\sim}{F}_B(r) \sim \left\{ \left(\frac{2r}{\nu}\right)^{-\nu} e^{\frac{r}{\nu}} - \left(\frac{2r}{\nu}\right)^{\nu} e^{-\frac{r}{\nu}}\,\underset{\sim}{\mathcal{B}} \right\} \tag{2.30}$$

But the physical solution must not contain divergent elements. It is only possible to find physical solution for particular energies called eigen energies . It is then possible to find a n-column matrix $\underset{\sim}{M}$ so that

$$\underset{\sim}{\mathcal{B}}^{-1}\,\underset{\sim}{M} = 0 \tag{2.31}$$

Then the column matrix physical solution $\underset{\sim}{P}(r)$ is equal to :

$$\underset{\sim}{P}(r) = -\underset{\sim}{F}_B\,\underset{\sim}{\mathcal{B}}^{-1}\underset{\sim}{M} = \left(\frac{2r}{\nu}\right)^{\nu} e^{-\frac{r}{\nu}}\,\underset{\sim}{M} \qquad (2.32)$$

2-6 Normalisation

In order to use the wave functions in a perturbation problem we need to know the normalisation of these wave functions For bound state we want orthonormalised functions i.e.

$$\int \Psi_A^*(x_1, x_2)\,\Psi_{A'}(x_1, x_2) = \delta \qquad (2.33)$$

where $\delta = 0$ if the wave functions correspond to different energies and $\delta = 1$ for the same eigen-energy . We shall prove in Chapter IV that (2.33) is satisfied for

$$\underset{\sim}{M} = K\,\underset{\sim}{X} \qquad (2.34)$$

where $K = \{\nu^2\Gamma(\ell+\nu+1)\Gamma(\nu-\ell)\}^{-1/2}$ and $\underset{\sim}{X}^T\underset{\sim}{X} = 1$
($\underset{\sim}{X}^T$ is the transpose matrix of $\underset{\sim}{X}$)

In the case of all open channels we obtain, using Green theorem (see Mott and Massey (1965)), from the definition of $\underset{\sim}{F}(\underset{\sim}{S}, r)$ that

$$\int_0^\infty dr\;\underset{\sim}{F}^+(\underset{\sim}{S}, r)\,\underset{\sim}{F}(\underset{\sim}{S}', r) = 2\pi\,\delta(E-E') \qquad (2.35)$$

where $\underset{\sim}{S}$ and $\underset{\sim}{S}'$ are the scattering matrices corresponding to the energies E and E' .

For closed and open channels the same relation holds with $\underset{\sim}{\mathcal{J}}$ and $\underset{\sim}{\mathcal{J}}'$.

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CHAPTER III

Perturbation of the electron-ion system by the radiation field

The time dependent perturbation theory is a powerful approximation for application in problems dealing with the radiation field. Many such applications are mentionned by Heitler (1954). For transitions between bound states the method gives a reliable theory for the natural line breadth (Wigner and Weisskopf, 1930). Davies and Seaton (1969) generalised the former theory to the case of transitions from free to bound electrons. Their paper is summarised in this chapter.

3-1 Time dependent perturbation theory

The idea is to consider that before a time $t = t_0$ there is no perturbation.

If we consider only transitions between bound states, ignoring the continuum, we can expend the wave function as follow

$$\Psi(t) = \sum_n b_n(t)\, \psi_n\, e^{-iE_n t} \qquad (3.1)$$

where $\psi_n e^{-iE_n t}$ are normalised eigen-solutions of the time-dependent Hamiltonian before $t = t_0$. The initial conditions are $b_i(t_0) = 1$, $b_j(t_0) = 0$ for $j \neq i$; the system is in the state ψ_i.
By introducing (3.1) in the Hamiltonian equation

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \qquad (3.2)$$

we obtain for $b_n(t)$ a set of time coupled equations. When t increases to infinity the system tends to equilibrium. At the limit, $t=+\infty$, the expected results are obtained : $b_n(\infty)$ represents the probability to be in the state n after the perturbation.

The same method can be applied for the continuum by changing (3.1) into the integral

$$\Psi_{\Gamma_0}(t) = \sum_{\Gamma} \int dE \, \frac{1}{\sqrt{2\pi}} \, \psi_{\Gamma}(E) \, e^{-iEt} f_{\Gamma\Gamma_0}(E,t) \qquad (3.3)$$

$\psi_{\Gamma}(E)$ is the antisymmetric function defined by (2.10) to which corresponds $F_{\Gamma\Gamma'}(\underset{\sim}{S},r)$,(2.26). The coefficient $\frac{1}{\sqrt{2\pi}}$ has been introduced so that the function $\frac{1}{\sqrt{2\pi}}\psi_{\Gamma}(E)$ is normalised to the Dirac function in energy (see : (2.35)).

3-2 Initial conditions

At the time $t_0=0$ the colliding electron is far from the ion and can be described as a wave packet having a dispersion $\delta \ll 1$, around $r_2 = r_0$ and an energy $E = \tilde{E}_0$, ($r_0\delta$ being large). The electron-ion system is in the state Γ_0 , E is no more an eigen-value.

$$\left.\begin{aligned} &\Gamma_0 = (n_0\, l_0\, k_0\, l'_0\, S_0\, L_0\, M_{S_0}\, M_{L_0}) \\ &E = E^{+}_{n_0 l_0} + \frac{k_0^2}{2} \quad , \quad \tilde{E}_0 = E^{+}_{n_0 l_0} + \frac{\tilde{k}_0^2}{2} \end{aligned}\right\} \qquad (3.4)$$

The probability coefficient $f_{\Gamma}(E,t)$ for $t=t_0=0$ represents the wave packet as defined.

$$f_{\Gamma\Gamma_0}(E,0)=\frac{\delta(\Gamma,\Gamma_0)\left(\frac{2\delta^3}{\pi k_0}\right)^{1/2}\exp(ix_0)}{(k-\hat{k}_0)^2+\delta^2} \tag{3.5}$$

the definition of X_0 can be deduced from (2.17).

$f_{\Gamma\Gamma_0}(E,0)$ is normalised as :

$$\sum_{\Gamma}\int dE\,\left|f_{\Gamma\Gamma_0}(E,0)\right|^2=1 \tag{3.6}$$

and using (2.10) and (2.7) we obtain

$$\Psi_{\Gamma_0}(0)=\mathcal{A}\,\phi_{\Gamma_0}(x,\hat{x}_2\sigma_2)\,\frac{\delta^{1/2}}{\hat{r}_2}\exp\left(-i(x_0-\hat{x}_0)-|\hat{r}_2-r_0|\delta\right) \tag{3.7}$$

where $\mathcal{A}$ is the classical antisymmetrisation operator.

Then we have

$$\left(\Psi_{\Gamma_0}(0)\,\middle|\,\Psi_{\Gamma_0}(0)\right)=1 \tag{3.8}$$

3-3 Time coupled equations

The Hamiltonian for the interaction of the radiation field with an atom is , at the first order :

$$H=-\alpha\,\vec{A}\cdot\vec{P} \tag{3.9}$$

α is the fine structure constant, $\vec{A}$ the vector potential and $\vec{P}$ the momentum of the atomic electrons.

A multipole expansion of the radiation field can be done, (Rose,1955, and Shore & Menzel, 1968) after which only the dipole electric term is considered. Then the radiation field is quantized and we can calculate matrix elements between free states without a photon and bound states with a photon.

$$H_{\Gamma\Gamma'}(q,E) = \left(\frac{2\omega^3_{\Gamma'}\alpha^3}{3\pi}\right)^{1/2} \frac{1}{\sqrt{2\pi}} \frac{(\Gamma E \| \underset{\sim}{R} \| \Gamma')}{\sqrt{(2L+1)(2S+1)}} C^{L'1L}_{M'_L q M_L} \delta_{SS'} \delta_{M_S M_{S'}} \quad (3.10)$$

ΓE corresponds to an initial free state represented by the coupling Γ and the energy E. Similarly Γ' represents the final bound state.

During the interaction all the bound states plus photon must be considered, included those for an energy $\Omega \neq E$.

$$\Omega = E_{\Gamma'} + \omega_{\Gamma'} \quad (3.11)$$

where $\omega_{\Gamma'}$ is the photon energy. In the resonance energy region $\omega_{\Gamma'}$ is pratically constant compared to $(\Gamma E \| \underset{\sim}{R} \| \Gamma')$, so we shall neglect the slow dependence of $H_{\Gamma\Gamma'}$ over Ω.

Let us introduce the probability density $|g_{\Gamma'}(\Omega,t)|^2$ that a photon, with a frequency $\omega_{\Gamma'}$, has been emitted leaving the electron-ion system in the bound state Γ'. With this definition of $g_{\Gamma'}(\Omega,t)$, the former hypothesis and (3.3) the time coupled equations are :

$$\left.\begin{aligned} \frac{d}{dt}\, f_\Gamma(E,t) &= i\, e^{iEt} \sum_{\Gamma'} \int d\Omega\, \mathcal{H}_{\Gamma\Gamma'}(E)\, e^{-i\Omega t}\, g_{\Gamma'}(\Omega,t) \\ \frac{d}{dt}\, g_{\Gamma'}(\Omega,t) &= i\, e^{i\Omega t} \sum_{\Gamma} \int dE\, \mathcal{H}^{*}_{\Gamma\Gamma'}(E)\, e^{-iEt}\, f_\Gamma(E,t) \end{aligned}\right\} \quad (3.12)$$

where

$$H_{\Gamma\Gamma'}(q,E) = -\ \mathcal{H}_{\Gamma\Gamma'}(E)\,.\ C^{L'1L}_{M'_L q M_L}\, \delta_{SS'}\, \delta_{M_S M_S'} \qquad (3.13)$$

in the formula (3.10) and in the definition of $g_{\Gamma'}(\Omega,t)$ we do not specify M_L and M_S for the dipole interaction is a Racah tensor. If it is necessary to specify M_L , M_S the corresponding probability is $g_{\Gamma'}(\Omega,t)$ multiplied by $C^{L'1L}_{M'_L q M_L}\, \delta_{SS'}\, \delta_{M_S M_S'}$. $\mathcal{H}_{\Gamma\Gamma'}$ is called the reduced tensor component.

For simplicity we shall use matrix algebra. Let's introduce $\underset{\sim}{f}(E,t)$ and $\underset{\sim}{g}(\Omega,t)$ which represent respectively the n-column matrix of the $f_\Gamma(E,t)$ and the p-column matrix of the $g_{\Gamma'}(\Omega,t)$ ("n" corresponds to the number of channels for the free solutions and "p" is the number of bound states into which the system may recombine after photo-emission). We have also to introduce $\dot{\underset{\sim}{f}}(E,t)$ and $\dot{\underset{\sim}{g}}(\Omega,t)$ for the $\frac{d}{dt} f_\Gamma(E,t)$ and $\frac{d}{dt} g_{\Gamma'}(\Omega,t)$. $\mathcal{H}(E)$ and $\mathcal{H}^+(E)$ represent the (n,p) matrix of the $\mathcal{H}_{\Gamma\Gamma'}(E)$ and the (p,n) matrix Hermitian conjuguate of $\mathcal{H}(E)$.

Then we have

$$\left.\begin{aligned} \dot{\underset{\sim}{f}}(E,t) &= i\, e^{iEt}\, \underset{\sim}{\mathcal{H}}(E) \int d\Omega\ e^{-i\Omega t}\, \underset{\sim}{g}(\Omega,t) \\ \dot{\underset{\sim}{g}}(\Omega,t) &= i\, e^{i\Omega t} \int dE\ \mathcal{H}^{+}(E)\, e^{-iEt}\, \underset{\sim}{f}(E,t) \end{aligned}\right\} \quad (3.14)$$

For convenience in the calculus Davies and Seaton introduced the following matrices :

$$\left.\begin{aligned} \underset{\sim}{F}(t) &= i\int dE\, \underset{\sim}{\mathcal{H}}^{+}(E)\; e^{-iEt}\, \underset{\sim}{f}(E,t) \\ \underset{\sim}{G}(t) &= i\int d\Omega\;\; e^{-i\Omega t}\; \underset{\sim}{g}(\Omega,t) \end{aligned}\right\} \qquad (3.15)$$

Then

$$\left.\begin{aligned} e^{-iEt}\, \underset{\sim}{\dot{f}}(E,t) &= \underset{\sim}{\mathcal{H}}(E)\; \underset{\sim}{G}(t) \\ e^{-i\Omega t}\; \dot{g}(\Omega,t) &= \underset{\sim}{F}(t) \end{aligned}\right\} \qquad (3.16)$$

3-4 Dielectronic recombination

Now in the case of dielectronic recombination

$$\underset{\sim}{g}(\Omega,0) = 0 \qquad (3.17)$$

(For photoionisation initial condition see 3-8)

By integrating the two equations (3.16) we have

$$\left.\begin{aligned} \underset{\sim}{f}(E,t) &= \underset{\sim}{\mathcal{H}}(E)\int_0^t d\tau\, e^{iE\tau}\, G(\tau) + f(E,0) \\ g(\Omega,t) &= \int_0^t d\tau\;\, e^{i\Omega\tau}\;\, F(\tau) \end{aligned}\right\} \qquad (3.18)$$

Then by substituing (3.18) into (3.15)

$$\underset{\sim}{F}(t) = i\int dE\, \underset{\sim}{\mathcal{H}}^{+}(E)\, e^{-iEt}\left\{ \underset{\sim}{\mathcal{H}}(E)\int_0^t d\tau\, e^{iE\tau}\, \underset{\sim}{G}(\tau) + \underset{\sim}{f}(E,0)\right\}$$

$$\underset{\sim}{G}(t) = i\int d\Omega\, e^{-i\Omega t}\int_0^t d\tau\, e^{i\Omega\tau}\, \underset{\sim}{F}(\tau) \tag{3.19}$$

By interchanging the order of integration and using the relation

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\Omega\, e^{i\Omega x} \tag{3.20}$$

we obtain

$$\underset{\sim}{G}(t) = 2\pi i\int_0^t \delta(\tau - t)\, F(\tau)\, d\tau = \pi i\, F(t) \tag{3.21}$$

(3.21) contains the hypothesis that $\underset{\sim}{\mathcal{H}}(E)$ is independant of Ω .

Now from (3.18) and (3.21) we get

$$\underset{\sim}{f}(E,t) = i\pi\, \underset{\sim}{\mathcal{H}}(E)\, g(E,t) + \underset{\sim}{f}(E,0) \tag{3.22}$$

In the ~~next~~ following part we shall derive the formula for $g(E,\infty)$:
From (3.18),(3.19) and (3.21) we have

$$\underset{\sim}{F}(t) = \int dE\, \underset{\sim}{\mathcal{H}}^{+}(E)\, e^{-iEt}\left\{ i\underset{\sim}{f}(E,0) - \pi\underset{\sim}{\mathcal{H}}(E)\int_0^t d\tau\, e^{iE\tau}\, \underset{\sim}{F}(\tau)\right\} \tag{3.23}$$

We define the Laplace transform of $\underset{\sim}{F}(t)$ as

$$\underset{\sim}{\phi}(s) = \int_0^\infty dt\, e^{-st}\, \underset{\sim}{F}(t) \tag{3.24}$$

We have $$g(\Omega,\infty) = \lim_{\epsilon\to 0} \phi(-i\Omega+\epsilon) \qquad (\epsilon>0)$$

By integrating (3.23) we obtain

$$\left\{ 1 + \underset{\sim}{L}(s) \right\} \underset{\sim}{\phi}(s) = \underset{\sim}{M}(s) \tag{3.25}$$

where

$$\left.\begin{aligned} \underset{\sim}{L}(s) &= \pi \int dE\, \frac{\underset{\sim}{\mathcal{H}}^{+}(E)\, \underset{\sim}{\mathcal{H}}(E)}{s+iE} \\ \underset{\sim}{M}(s) &= i \int dE\, \frac{\underset{\sim}{\mathcal{H}}^{+}(E)\, \underset{\sim}{f}(E,0)}{s+iE} \end{aligned}\right\} \tag{3.26}$$

Using the definition (3.5) of $\underset{\sim}{f}(E,0)$ Davies and Seaton proved that

$$\lim_{\substack{\epsilon\to 0 \\ (\epsilon>0)}} \underset{\sim}{M}(-i\Omega+\epsilon) = 2i\pi\, \underset{\sim}{\mathcal{H}}^{+}(\Omega)\, \underset{\sim}{f}(\Omega,0) \tag{3.27}$$

thus

$$\underset{\sim}{g}(\Omega,\infty) = 2i\pi \left\{ 1 + \underset{\sim}{Z}(\Omega) \right\}^{-1} \underset{\sim}{\mathcal{H}}^{+}(\Omega)\, \underset{\sim}{f}(\Omega,0) \tag{3.28}$$

Hence from (3.22) we have

$$f(E,\infty) = \left[1 - 2\pi^2 \underset{\sim}{\mathcal{H}}(E) \left\{ 1 + \underset{\sim}{Z}(E) \right\}^{-1} \underset{\sim}{\mathcal{H}}^{+}(E) \right] \underset{\sim}{f}(E,0) \tag{3.29}$$

where $$Z(\Omega) = \lim_{\substack{\epsilon\to 0 \\ (\epsilon>0)}} \frac{\pi}{i} \int dE\, \frac{\mathcal{H}^{+}(E)\, \mathcal{H}(E)}{E-\Omega-i\epsilon} \tag{3.30}$$

3-5 Generalised $\mathcal{S}$ matrix

In collision theory the element $\mathcal{S}_{\Gamma'\Gamma}$ of the $\underset{\sim}{\mathcal{S}}$ matrix is the probability that an electron arriving in the channel Γ leaves in the channel Γ'. Therefore if we neglect the radiation field interaction we have

$$\underset{\sim}{\mathcal{S}} \; \underset{\sim}{f}(E,0) \tag{3.31}$$

This is the row matrix of the probability flux of outgoing electrons corresponding to the initial condition $\underset{\sim}{f}(E,0)$.

If the radiation field interaction is included (3.31) becomes

$$\underset{\sim}{\mathcal{S}} \; \underset{\sim}{f}(E,\infty) \tag{3.32}$$

By using (3.29), (3.32) can be expressed in a function of $\underset{\sim}{f}(E,0)$

$$\underset{\sim}{\mathcal{S}} \left\{ 1 - 2\pi^2 \underset{\sim}{\mathcal{H}} \left[1 + \underset{\sim}{Z} \right]^{-1} \underset{\sim}{\mathcal{H}}^+ \right\} \underset{\sim}{f}(E,0) \tag{3.33}$$

We define a generalised $\mathcal{S}$ matrix which includes photo-interaction. Then in the case of collision scattering without photon emission the old $\underset{\sim}{\mathcal{S}}$ matrix is modified to :

$$\underset{\sim}{\mathcal{S}}^{(e,c)} = \underset{\sim}{\mathcal{S}} \left\{ 1 - 2\pi^2 \underset{\sim}{\mathcal{H}} \left[1 + \underset{\sim}{Z} \right]^{-1} \underset{\sim}{\mathcal{H}}^+ \right\} \tag{3.34}$$

The difference of flux between (3.31) and (3.32) corresponds to the recombination flux into bound states with the emission of a photon.

$$\underset{\sim}{g}(E,\infty) = 2\pi i \left[1 + \underset{\sim}{Z} \right]^{-1} \underset{\sim}{\mathcal{H}}^+ \underset{\sim}{f}(E,0) \tag{3.35}$$

This gives the $\underset{\sim}{S}$ matrix for photo-recombination as

$$\underset{\sim}{S}^{(p,e)} = 2\pi i \left[1 + \underset{\sim}{Z} \right]^{-1} \underset{\sim}{\mathcal{H}}^{+} \qquad (3.36)$$

3-6 Unitarity of the generalised S matrix

In their paper Davies and Seaton proved the useful formula

$$\underset{\sim}{Z} + \underset{\sim}{Z}^{+} = 2\pi^{2} \underset{\sim}{\mathcal{H}}^{+} \underset{\sim}{\mathcal{H}} \qquad (3.37)$$

Using (3.37) it is easy to check the unitarity of the generalised $\underset{\sim}{S}$ matrix

$$\underset{\sim}{S}^{(e,e)+} \underset{\sim}{S}^{(e,e)} + \underset{\sim}{S}^{(p,e)+} \underset{\sim}{S}^{(p,e)} = 1 \qquad (3.38)$$

3-7 Commentary on the former method

In the case of dielectronic recombination the time-dependant perturbation theory is very suitable since at the beginning the colliding electron and the ion are far apart and that the electron is in the static asymptotic coulomb potential of the ion. But this reason is not enough for determining the choice between first order perturbation theory and time dependant perturbation theory. The difference between these two theories is that the first doesn't conserve the flux of electron when the second does. This is particularly important for large quantum number resonance (say resonance "n") where the probability of capture in the first theory is constant with n, in the second theory it decreases rapidly. And has for inconvenient to give for the first theory a divergent expression for the dielectronic recombination rate.

3-8 Photoionisation

The difference between dielectronic recombination and photoionisation is found in the initial boundary condition : i.e.

$$\underset{\sim}{f}(E,0) = 0 \tag{3.39}$$

instead of (3.17).

By integrating the two equations ,(3.16), we have

$$\begin{aligned} \underset{\sim}{f}(E,t) &= \underset{\sim}{\mathcal{H}}(E) \int_0^t d\tau \, e^{iE\tau} \underset{\sim}{G}(\tau) \\ \underset{\sim}{g}(\Omega,t) &= \int_0^t d\tau \, e^{i\Omega\tau} \underset{\sim}{F}(\tau) + \underset{\sim}{g}(\Omega,0) \end{aligned} \tag{3.40}$$

and by substituing (3.40) in (3.15)

$$\underset{\sim}{G}(t) = i \int d\Omega \, e^{-i\Omega t} \left[\int_0^t d\tau \, e^{i\Omega\tau} \underset{\sim}{F}(\tau) + \underset{\sim}{g}(\Omega,0) \right] \tag{3.41}$$

this gives

$$\underset{\sim}{G}(t) = \pi i \, \underset{\sim}{F}(t) + i \int d\Omega \, e^{-i\Omega t} \underset{\sim}{g}(\Omega,0) \tag{3.42}$$

Now using (3.40) and (3.42)

$$\underset{\sim}{f}(E,t) = \pi i\, \underset{\sim}{\mathcal{H}}(E) \int_0^t d\tau\, e^{iE\tau} \underset{\sim}{F}(\tau) + i\, \underset{\sim}{\mathcal{H}}(E) \int_0^t d\tau\, e^{iE\tau} \int d\Omega\, e^{-i\Omega\tau} \underset{\sim}{g}(\Omega,0) \qquad (3.43)$$

and by using also the same kind of argument as Davies and Seaton we finally obtain

$$\underset{\sim}{f}(E,\infty) = i\pi\, \underset{\sim}{\mathcal{H}}(E) \Big(\underset{\sim}{g}(E,\infty) + \underset{\sim}{g}(E,0) \Big) \qquad (3.44)$$

and

$$\underset{\sim}{g}(\Omega,\infty) = \Big(1 - \underset{\sim}{Z}(\Omega) \Big)\Big(1 + \underset{\sim}{Z}(\Omega) \Big)^{-1} \underset{\sim}{g}(\Omega,0) \qquad (3.45)$$

this gives from (3.44)

$$\underset{\sim}{f}(E,\infty) = 2\pi i\, \underset{\sim}{\mathcal{H}}(E) \Big(1 + \underset{\sim}{Z}(E) \Big)^{-1} \underset{\sim}{g}(E,0) \qquad (3.46)$$

The symmetry of the two processes is evident by comparing (3.28) and (3.46)

As in 3-5 we shall now define new elements of the generalised $\underset{\sim}{S}$ matrix :

$$\underset{\sim}{S}^{(P,P)} = \Big(1 - \underset{\sim}{Z} \Big)\Big(1 + \underset{\sim}{Z} \Big)^{-1} \qquad (3.47)$$

and

$$\underset{\sim}{S}^{(e,p)} = 2\pi i \, \underset{\sim}{S} \, \underset{\sim}{\mathcal{H}} \left(1 + \underset{\sim}{Z} \right)^{-1} \tag{3.48}$$

The generalised $\underset{\sim}{S}$ matrix is now completely defined

$$\underset{\sim}{S}^{G} = \begin{pmatrix} \underset{\sim}{S}^{(e,e)} & \underset{\sim}{S}^{(e,p)} \\ \underset{\sim}{S}^{(p,e)} & \underset{\sim}{S}^{(p,p)} \end{pmatrix} \tag{3.49}$$

$\underset{\sim}{S}^{G}$ is a (n+p,n+p) matrix .

From (3.34),(3.36),(3,47) and (3.48) it is easy to deduce

$$\left(\underset{\sim}{S}^{G}\right)^{+} \underset{\sim}{S}^{G} = \underset{\sim}{S}^{G} \left(\underset{\sim}{S}^{G}\right)^{+} = 1 \tag{3.50}$$

Hence the $\underset{\sim}{S}^{G}$ matrix is unitary (but not symmetric) .

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CHAPTER IV

Study of the collision resonance structure for $He^+ + e^-$

In order to represent a resonance curve by a mathematical formula, Wigner (1946) studied the solutions of the quantum theory equations in function of energy. By fixing appropriate boundary conditions he succeeded in developing the solutions as a Taylor series in the energy. From there Wigner and Eisenbud (1947) defined the "R matrix theory" from which in turn, much later, Gailitis (1963) deduced equivalent results to those obtained in this chapter.

At the same time Jost (1947) studied the analyticity of the scattering $\underset{\sim}{S}$ matrix as a function of energy. He pointed out that the equations had already been studied by Poincare (1884) who had proved the analyticity of the solutions satisfying boundary conditions for more general differential equations.

Later Ham (1955), who was interested by the possibility of numerical results, applied the analytical properties to the case of a short range potential combined with a Coulomb field. Following Ham's idea Seaton (1958) proved the possibility of extrapolating the quantum defect to the elastic phase shift.

In 1966 Seaton generalised the former theory to obtain numerical results for the radial coupled equations problem. Hence in 1969 he came back to the Wigner problem finding a more accurate resonance formula for ion-electron collision resonance.

The formula contains unknown parameters that are slowly varying with energy and can be estimated by solving the coupled equations for a few energies.

Seaton's method gives very good results for many practical cases. But in the case of $He^+ + e^-$,due to the degeneracy of the "2s" and "2p" states, the long range interaction apart from the Coulomb potential are too important to neglect as Seaton's theory does. To improve the method for this case Bely (1966) used a diagonalisation method which includes the most important long range potential into the centrifugal terms. The same idea had already been used by Seaton (1961) for improving the Born Approximation.

Bely's formulation of the problem is difficult to use therefore in this chapter we shall try to simplify it by adding a few mathematical hypothesis that are justified in practice. This shall also allow us to deduce a resonance formula similar to Seaton (1969). In the next chapter we shall use the former formula applied to the dielectronic recombination problem.

4-2 Coupled radial equations

We shall be interested only by the energy region around the first threshold of He^+ excitation where it should be a good approximation to include in (2.10) only three ionic functions corresponding to the "1s","2s" and "2p" states. For a total angular momentum $L = 0$ the system reduces to three equations and for $L \neq 0$ to four .

The following initial and final channels correspond to the equations (2.12) :

$$\Gamma_1 = (1s\ k_1,\ l_1 = L,\ LSM_LM_S)$$

$$\Gamma_2 = (2s\ k_2,\ l_2 = L,\ LSM_LM_S)$$

$$\Gamma_3 = (2p\ k_3,\ l_3 = L+1,\ LSM_LM_S)$$

$$\Gamma_4 = (2p\ k_4,\ l_4 = L-1,\ LSM_LM_S)$$

(for $L = 0$, Γ_4 doesn't exist)

The "2s" and "2p" states are degenerate for He$^+$: $k_2 = k_3 = k_4$

Using the indice i for representing Γ_i (2.12) becomes :

$$\left\{\frac{d^2}{dr^2} - \frac{l_i(l_i+1)}{r^2} + \frac{2}{r} + \epsilon_i\right\} F_{ij}(r) = \sum_k U_{ik}(r) F_{kj}(r) \quad (4.1)$$

where $\epsilon_i = k_i^2$. j represents the initial channel and i the final channel.

4-3 Analyticity

As we wrote in (2.18) we consider only the solutions having the following physical property

$$F_{ij}(0) = 0 \qquad (4.2)$$

The solution vector space has the dimension $n = 4$ or 3. Now if we take $F_{ij}(E,r)$ analytic in energy E in the neighbourhood of $r = 0$ it can be proved (Ham,1955, and Seaton,1966) that $F_{ij}(E,r)$ is analytic for any finite r.

Let $\underset{\sim}{F}(E,r)$ be a matrix made of n independant column matrix solutions satisfying the former condition. They form a basis set and any other basis set can be obtained from $\underset{\sim}{F}(E,r)$ by a matrix transformation.

4-4 Asymptotic potential

For r increasing $U_{ik}(r)$ tends to zero. It is possible to expand $U_{ik}(r)$ as follow :

$$U_{ik}(r) = \sum_{m=2}^{\infty} \frac{\alpha_{ik}^{(m)}}{r^m} \qquad r \geqslant r_0 \tag{4.3}$$

In general $\alpha_{ik}^{(m)}$ is small and in Seaton (1966) and (1969) it is assumed that for $r \geqslant r_0$ $U_{ik}(r) = 0$.

The states "2s" and "2p" being degenerate then the dipole interaction between these states is very strong and the former hypothesis is not valid at all. Following Bely (1966) (but also Seaton (1961) and Gailitis (1963)) we shall not neglect the elements $\alpha_{ik}^{(2)}$ for i and k equal to 2,3,4. All the other interactions (for $m > 2$ and also $\alpha_{k1}^{(2)}$ for $k \neq 1$) will be neglected.

For $r \geqslant r_0$ (4.1) takes the following form :

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r} + \epsilon \right\} \underset{\sim}{F}(r) = \frac{1}{r^2} \underset{\sim}{A} \, \underset{\sim}{F}(r) \qquad (4.4)$$

where

$$\underset{\sim}{A} = \begin{pmatrix} \ell_1(\ell_1+1) & 0 & 0 & 0 \\ 0 & \ell_2(\ell_2+1) & \alpha_{32} & \alpha_{42} \\ 0 & \alpha_{32} & \ell_3(\ell_3+1) & 0 \\ 0 & \alpha_{42} & 0 & \ell_4(\ell_4+1) \end{pmatrix} \qquad (4.5)$$

$\underset{\sim}{A}$ being symmetric we can diagonalise it thus

$$\underset{\sim}{O}^T \underset{\sim}{A} \, \underset{\sim}{O} = a \qquad (4.6)$$

where $\underset{\sim}{O}^T$ is the transpose matrix of $\underset{\sim}{O}$.

$$\underset{\sim}{O}^T \underset{\sim}{O} = \underset{\sim}{O} \, \underset{\sim}{O}^T = 1 \qquad (4.7)$$

and a is diagonal .

The first row and first column of $\underset{\sim}{A}$ being already diagonalised the first row and first column of $\underset{\sim}{O}$ will be zero excepted $O_{11} = 1$.

The former property of the matrix $\underset{\sim}{O}$ is fundamental in that

$$\underset{\sim}{O}\,\epsilon = \epsilon\,\underset{\sim}{O}$$

$$\underset{\sim}{O}^T\,\epsilon = \epsilon\,\underset{\sim}{O}^T$$

Now let's define

$$\underset{\sim}{G} = \underset{\sim}{O}^T\,\underset{\sim}{F} \qquad (4.8)$$

we obtain from (4.4)

$$r^2\left\{\frac{d^2}{dr^2} + \frac{2}{r} + \epsilon\right\}\underset{\sim}{G} = a\,\underset{\sim}{G} \qquad r \geq r_0 \qquad (4.9)$$

by defining λ_i from $a_{ii} = \lambda_i(\lambda_i+1)$ the equation (4.9) takes the coulombic form

$$\left\{\frac{d^2}{dr^2} - \frac{\lambda_i(\lambda_i+1)}{r^2} + \frac{2}{r} + \epsilon_i\right\} G_{ij}(r) = 0 \qquad r \geq r_0 \qquad (4.10)$$

λ_i is not necessary integer and can be real or complex having the form $\lambda_i = -\frac{1}{2} + i\bar{\lambda}$ where $\bar{\lambda}$ is real.

4-5 Solutions of the coulombic equation

a) Analytic solutions

In this part we shall study the solutions of

$$\left\{\frac{d^2}{dr^2} - \frac{\lambda_i(\lambda_i+1)}{r^2} + \frac{2}{r} + \epsilon_i\right\} y(\epsilon,\lambda,r) = 0 \qquad (4.11)$$

for any r , λ being real or $\lambda = -\frac{1}{2} + i\bar{\lambda}$ with $\bar{\lambda}$ real.

In Seaton's paper (1958) he defined for any $\epsilon \; \lambda \; r$ two functions analytic in energy ϵ :

$$\left.\begin{aligned} y_1(\epsilon\lambda r) &= \frac{\kappa^{\lambda+1}}{\Gamma(2\lambda+2)} \, M_{\kappa,\lambda+\frac{1}{2}}\left(\frac{2r}{\kappa}\right) \\ y_2(\epsilon\lambda r) &= \frac{\kappa^{-\lambda}}{\Gamma(-2\lambda)} \, M_{\kappa,-\lambda-\frac{1}{2}}\left(\frac{2r}{\kappa}\right) \end{aligned}\right\} \qquad (4.12)$$

where $\epsilon = k^2 = -\frac{1}{\kappa^2}$ and $M_{\kappa,m}(\rho)$ had been defined by Whittaker and Watson (1946).

For $\epsilon > 0$ we take $\kappa = i\gamma$ with $\gamma > 0$ and for $\epsilon < 0$ $\kappa = \nu$ with $\nu > 0$.

y_1 and y_2 are linearly independant excepted for $\lambda = \ell$, ℓ integer :

$$y_2(\epsilon \ell r) = -A(\epsilon \ell) \, y_1(\epsilon \ell r) \qquad (4.13)$$

with

$$A(\epsilon\lambda) = \frac{\Gamma(\kappa+\lambda+1)}{\kappa^{2\lambda+1}\,\Gamma(\kappa-\lambda)} \qquad (4.14)$$

Studying $A(\epsilon\lambda)$ for λ real and $\lambda = -\frac{1}{2} + i\bar{\lambda}$ we find that $A(\epsilon\lambda)$ is slowly varying with energy in the neighbourhood of $\epsilon = 0$ (for more details see Appendix 1)

b) Asymptotic form

The physical solutions have asymptotic boundary conditions (see (2.21) and (2.23) .....)

We shall study $y_1(\epsilon\lambda r)$ and $y_2(\epsilon\lambda r)$ for r large so as to relate them to these physical solutions.

The asymptotic form of the Whittaker $M_{\kappa,m}(\rho)$ function is found in Slater (1960).

1) <u>ϵ negative</u>

For $\kappa = \nu$ a difficulty arises : the function $M_{\nu,m}(\frac{2r}{\nu})$ is double valued and the asymptotic form of both of them is complex. But we know by developing $M_{\nu m}(\frac{2r}{\nu})$ in a series, for λ real, that $M_{\nu m}(\frac{2r}{\nu})$ is real for any finite r . Further we find , in this case, that the imaginary part of Slater's asymptotic formula must be neglected compared to the real divergent part. Hence we deduce that the imaginary part, for λ real, is meaningless.

For $\lambda = -\frac{1}{2} + i\bar{\lambda}$ the problem is still not solved. But it can be seen that $M_{\nu m}(\frac{2r}{\nu})$ is given by the same expression for λ real or $\lambda = -\frac{1}{2} + i\bar{\lambda}$. We shall suppress the corresponding part. We check that this term is convergent to zero and that the formula obtained after this operation is not in contradiction with any relation between y_1 and y_2 .

Thus for any λ real or $\lambda = -\frac{1}{2} + i\bar{\lambda}$ we have :

$$\left.\begin{aligned} y_1(\epsilon\lambda r) &\sim \nu^{\lambda+1}\left[\frac{\xi}{\Gamma(\lambda+1-\nu)} + \frac{\Theta\cos\pi(\nu-\lambda-1)}{\Gamma(\lambda+1+\nu)}\right] \\ y_2(\epsilon\lambda r) &\sim \nu^{-\lambda}\left[\frac{\xi}{\Gamma(-\lambda-\nu)} + \frac{\Theta\cos\pi(\nu+\lambda)}{\Gamma(-\lambda+\nu)}\right] \end{aligned}\right\} \quad (4.15)$$

(the sine and sosine are defined for complex arguments)

where

$$\left.\begin{aligned} \xi &= e^{\frac{r}{\nu}} \left(\frac{2r}{\nu}\right)^{-\nu} \\ \theta &= e^{-\frac{r}{\nu}} \left(\frac{2r}{\nu}\right)^{\nu} \end{aligned}\right\} \qquad (4.16)$$

Let's introduce

$$K(\nu,\lambda) = \frac{1}{\nu\left\{\Gamma(\nu+\lambda+1)\,\Gamma(\nu-\lambda)\right\}^{1/2}} \qquad (4.17)$$

$K(\nu,\lambda)$ is real and positive for any λ real or $\lambda = -\frac{1}{2} + i\bar{\lambda}$.

For $\lambda = -\frac{1}{2} + i\bar{\lambda}$:

$$K(\nu,\lambda) = \frac{1}{\nu\left|\Gamma(\nu+\frac{1}{2}-i\bar{\lambda})\right|} \qquad (4.18)$$

(for more details about $K(\nu,\lambda)$ see Appendix 2)

Let's define

$$\left.\begin{aligned} s^{\circ} &= \sqrt{\frac{\pi}{2}} \left(\frac{y_1 A^{1/2} - y_2 A^{-\frac{1}{2}}}{2\cos\pi\lambda}\right) \\ c^{\circ} &= -\sqrt{\frac{\pi}{2}} \left(\frac{y_1 A^{1/2} + y_2 A^{-1/2}}{2\sin\pi\lambda}\right) \end{aligned}\right\} \qquad (4.19)$$

from (4.15) it is easy to deduce :

$$\left.\begin{aligned} s^{\circ} &\underset{r\to\infty}{\sim} \sqrt{\frac{\pi}{2}} \left[\frac{\xi}{\pi K \nu^{1/2}} \sin\pi\nu - \theta K \nu^{3/2} \cos\pi\nu\right] \\ c^{\circ} &\underset{r\to\infty}{\sim} \sqrt{\frac{\pi}{2}} \left[\frac{\xi}{\pi K \nu^{1/2}} \cos\pi\nu + \theta K \nu^{3/2} \sin\pi\nu\right] \end{aligned}\right\} \qquad (4.20)$$

The functions s^0 and c^0 are linearly independant coulombic solutions for any λ (real or $\lambda = -\frac{1}{2} + i\bar{\lambda}$). They are not analytic but vary slowly with ϵ since $A(\epsilon\lambda)$ is slowly varying with ϵ. For $\lambda = \ell$ multiplying s^0 and c^0 by $(-1)^l$ we obtain the solutions defined by Eissner et al. (1969).

2) <u>ϵ positive</u>

α) <u>λ real</u>

From the asymptotic form of $M_{\kappa m}(\rho)$ we obtain

$$\left.\begin{aligned} y_1 &\sim \frac{2e^{-\frac{\pi\gamma}{2}}\gamma^{\lambda+1}}{|\Gamma(\lambda+1+i\gamma)|}\sin\left\{kr - \frac{\lambda\pi}{2} + \gamma\log 2kr + \arg\Gamma(\lambda+1-i\gamma)\right\} \\ y_2 &\sim \frac{2e^{-\frac{\pi\gamma}{2}}}{\gamma^{\lambda}|\Gamma(-\lambda-i\gamma)|}\sin\left\{kr + \frac{(\lambda+1)\pi}{2} + \gamma\log 2kr + \arg\Gamma(-\lambda-i\gamma)\right\} \end{aligned}\right\} \quad (4.21)$$

By neglecting $e^{-2\pi\gamma}$ compared to 1 we have

$$\Gamma(i\gamma-\lambda)\,\Gamma(1+\lambda-i\gamma) \simeq \frac{2\pi}{e^{\pi\gamma}\,e^{\frac{i\pi}{2}(2\lambda+1)}} \qquad (4.22)$$

Then

$$\left.\begin{aligned} s^0 &\sim \gamma^{1/2}\sin\left\{kr + \frac{\lambda\pi}{2} + \gamma\log 2kr + \arg\Gamma(\lambda+1-i\gamma)\right\} \\ c^0 &\sim \gamma^{1/2}\cos\left\{kr + \frac{\lambda\pi}{2} + \gamma\log 2kr + \arg\Gamma(\lambda+1-i\gamma)\right\} \end{aligned}\right\} \quad (4.23)$$

β) $\lambda = -\frac{1}{2} + i\bar{\lambda}$

Using the same approximation ($e^{-2\pi\gamma} \ll 1$) we have

$$\left.\begin{aligned} s_0 &\sim \gamma^{1/2} \sin\left\{kr + \gamma \log 2kr - \frac{\pi}{4} + \varphi(\bar{\lambda},\gamma)\right\} \\ c_0 &\sim \gamma^{1/2} \cos\left\{kr + \gamma \log 2kr - \frac{\pi}{4} + \varphi(\bar{\lambda},\gamma)\right\} \end{aligned}\right\} \tag{4.24}$$

with

$$\varphi(\bar{\lambda},\gamma) = \frac{\arg\Gamma\left(\frac{1}{2} - i(\gamma+\bar{\lambda})\right) + \arg\Gamma\left(\frac{1}{2} - i(\gamma-\bar{\lambda})\right)}{2} \tag{4.25}$$

3) $\epsilon = 0$

At the threshold, $\epsilon = 0$, the coulombic solutions becomes Bessel functions (see Seaton (1958) formulae (18),(19)) By using the asymptotic form of the Bessel functions we deduce

$$\left.\begin{aligned} y_1 &\sim \sqrt{\frac{2}{\pi}} \left(\frac{r}{2}\right)^{1/4} \sin\left(\sqrt{8r} - \lambda\pi - \frac{\pi}{4}\right) \\ y_2 &\sim \sqrt{\frac{2}{\pi}} \left(\frac{r}{2}\right)^{1/4} \sin\left(\sqrt{8r} + (\lambda+1)\pi - \frac{\pi}{4}\right) \end{aligned}\right\} \tag{4.26}$$

This gives

$$\left.\begin{aligned} s^0 &\sim \left(\frac{r}{2}\right)^{1/4} \sin\left(\sqrt{8r} - \frac{\pi}{4}\right) \\ c^0 &\sim \left(\frac{r}{2}\right)^{1/4} \cos\left(\sqrt{8r} - \frac{\pi}{4}\right) \end{aligned}\right\} \tag{4.27}$$

c) Commentary on s^0 and c^0

When we studied the asymptotic form we found it simple and convenient to define the solutions s^0 and c^0 : They are linearly independant for any λ .They are continuous on the variable λ (this will be particularly important in the case of collision ion-electron with large angular momentum when all the λ converge to integer) . These solutions are not analytic but slowly varying with energy. For $\epsilon \geqslant 0$, they are in quadrature of phase which is of fundamental importance in the following part, 4-7 .

4-6 Slowly varying matrices

The transformation from $\underset{\sim}{F}$ to $\underset{\sim}{G}$ is given by the matrix $\underset{\sim}{O}$ which is constant with energy . Hence the matrix $\underset{\sim}{G}$ will be, like $\underset{\sim}{F}$, analytic in energy.

We introduce the new set of coulombic solutions

$$\left. \begin{array}{l} s_1^* = (-1)^{l_1} s_1^0 \quad , \quad c_1^* = (-1)^{l_1} c_1^0 \\ s_i^* = s_i^0 \quad , \quad c_i^* = c_i^0 \quad \text{for } i=2,3,4 \end{array} \right\} \qquad (4.28)$$

The functions s_1^* and c_1^* are defined so as to coincide with the classical $\sin(x_1)$ and $\cos(x_1)$ where

$$x_1 = k_1 r - \frac{l_1 \pi}{2} + \gamma_1 \log 2 k_1 r + \arg \Gamma(l_1 + 1 - i\gamma_1)$$

For $r \geqslant r_0$ we expand $\underset{\sim}{G}$ on the slowly varying functions s^* and c^* :

$$G_{ij}(r) = s_i^* \mathcal{A}_{ij} + c_i^* \mathcal{B}_{ij} \tag{4.29}$$

$\mathcal{A}_{ij}$ and $\mathcal{B}_{ij}$ are then slowly varying matrix elements .

4-7 $\mathcal{R}$- matrix

The $\underset{\sim}{\mathcal{R}}$ matrix is defined as

$$\underset{\sim}{\mathcal{R}} = \underset{\sim}{\mathcal{B}}\,\underset{\sim}{\mathcal{A}}^{-1} \tag{4.30}$$

$\underset{\sim}{\mathcal{R}}$ is symmetric and real (see Appendix 3)

From (4.30) we see that $\underset{\sim}{\mathcal{R}}$ is also slowly varying with energy.

4-8 Resonance structure

a) General formula

The $\underset{\sim}{\mathcal{R}}$ matrix has the same properties as the reactance matrix, $\underset{\sim}{R}$ matrix, this will allow us to use the method developed by Seaton (1969).

We define

$$\underset{\sim}{\chi} = (1 + i\underset{\sim}{\mathcal{R}})(1 - i\underset{\sim}{\mathcal{R}})^{-1} \tag{4.31}$$

$\underset{\sim}{\mathcal{R}}$ being real and symmetric $\underset{\sim}{\chi}$ is unitary and symmetric.

$\underset{\sim}{\mathcal{R}}$ varying slowly, $\underset{\sim}{\chi}$ also varies slowly with energy. Corresponding to the $\underset{\sim}{S}$ matrix in Seaton (1969) let's define $\underset{\sim}{\Sigma}$ so that $\underset{\sim}{\Sigma} = \underset{\sim}{\chi}$ when all the channels are open .

$$\underset{\sim}{G}(\underset{\sim}{\Sigma}, r) \sim \phi^- - \phi^+ \underset{\sim}{\Sigma} \qquad (4.32)$$

where for $k_2^2 > 0$ (all channels opened) and j=1,2,3,4

$$\phi_j^+ = c_j^* + i s_j^* \quad , \quad \phi_j^- = c_j^* - i s_j^* \qquad (4.33)$$

and for $k_2^2 < 0$, j=2,3,4

$$\phi_j^{\pm} = \left(\frac{2r}{\nu_2}\right)^{\pm\nu_2} e^{\mp\frac{r}{\nu_2}} \qquad (4.34)$$

$\phi_1^{\pm}$ stays unchanged.

We can write $\underset{\sim}{\Sigma}$ as follow :

$$\underset{\sim}{\Sigma} = a\left(1 - T\underset{\sim}{\mathcal{R}}\right)\left(1 + C\underset{\sim}{\mathcal{R}}\right)^{-1} b \qquad (4.35)$$

The definition of a , b , T , C are given in table 4*1

Following Seaton (1969) we define

$$\underset{\sim}{Z} = \left(1 - T\underset{\sim}{\mathcal{R}}\right)\left(1 + C\underset{\sim}{\mathcal{R}}\right)^{-1} \qquad (4.36)$$

By eliminating $\underset{\sim}{\mathcal{R}}$ between (4.31) and (4.36) we have

$$\underset{\sim}{Z}\left\{(1+iC) + (1-iC)\underset{\sim}{\chi}\right\} = (1+iT)\chi + (1-iT) \qquad (4.37)$$

We partition $\underset{\sim}{Z}$, $\underset{\sim}{\chi}$, C and T in open and closed parts :

	$K_i = i\gamma_i$	$K_i = \nu_i$
a	1	$\frac{\sqrt{2\pi}}{i} K_i \nu_i^{3/2} \cos \pi\nu_i$
b	1	$\frac{i}{\sqrt{2\pi}} \frac{\pi K_i \nu_i^{1/2}}{\sin \pi\nu_i}$
T	$-i$	$\tan \pi\nu_i$
C	$-i$	$\cot \pi\nu_i$

TABLE 4*1

$$\underset{\sim}{Z} = \begin{pmatrix} \underset{\sim}{Z}_{oo} & \underset{\sim}{Z}_{oc} \\ \underset{\sim}{Z}_{co} & \underset{\sim}{Z}_{cc} \end{pmatrix} \qquad \underset{\sim}{\chi} = \begin{pmatrix} \underset{\sim}{\chi}_{oo} & \underset{\sim}{\chi}_{oc} \\ \underset{\sim}{\chi}_{co} & \underset{\sim}{\chi}_{cc} \end{pmatrix}$$

$$\underset{\sim}{C} = \begin{pmatrix} -i & 0 \\ 0 & c \end{pmatrix} \qquad \underset{\sim}{T} = \begin{pmatrix} -i & 0 \\ 0 & t \end{pmatrix} \tag{4.38}$$

we obtain from (4.37) four equations

$$\begin{aligned}
2\underset{\sim}{Z}_{oo} + \underset{\sim}{Z}_{oc}(1-ic)\underset{\sim}{\chi}_{co} &= 2\underset{\sim}{\chi}_{oo} \\
\underset{\sim}{Z}_{oc}\left[(1+ic) + (1-ic)\underset{\sim}{\chi}_{cc}\right] &= 2\underset{\sim}{\chi}_{oc} \\
2\underset{\sim}{Z}_{co} + \underset{\sim}{Z}_{cc}(1-ic)\underset{\sim}{\chi}_{co} &= (1+it)\underset{\sim}{\chi}_{co} \\
2\underset{\sim}{Z}_{cc}\left[(1+ic) + (1-ic)\underset{\sim}{\chi}_{cc}\right] &= (1-it) + (1+it)\underset{\sim}{\chi}_{cc}
\end{aligned} \tag{4.39}$$

By eliminating $\underset{\sim}{Z}_{oc}$ and $\underset{\sim}{Z}_{cc}$ between these equations we have

$$\left.\begin{aligned}
\underset{\sim}{Z}_{oo} &= \underset{\sim}{\chi}_{oo} - \underset{\sim}{\chi}_{oc}\left(\underset{\sim}{\chi}_{cc} - e^{-2\pi i\nu}\right)^{-1}\underset{\sim}{\chi}_{co} \\
\underset{\sim}{Z}_{co} &= (it-1)\left(\underset{\sim}{\chi}_{cc} - e^{-2\pi i\nu}\right)^{-1}\underset{\sim}{\chi}_{co}
\end{aligned}\right\} \tag{4.40}$$

where

$$e^{-2\pi i\nu} = \frac{(1-it)}{(1+it)} = -\frac{(1+ic)}{(1-ic)} \tag{4.41}$$

b) Degenerate closed channels

Since the closed channels are degenerate in the case of $He^+ + e^-$, $e^{-2\pi i\nu}$ is a multiple of the unit matrix

$\underset{\sim}{\chi}_{cc}$ being symmetric can be diagonalised thus :

$$\left.\begin{aligned} \chi_{cc} &= X\,\chi'_{cc}\,X^T \\ XX^T &= X^TX = 1 \end{aligned}\right\} \qquad (4.42)$$

Therefore we have

$$\left.\begin{aligned} \underset{\sim}{Z}_{oo} &= \underset{\sim}{\chi}_{oo} - \underset{\sim}{\chi}'_{oc}\left(\underset{\sim}{\chi}'_{cc} - e^{-2\pi i\nu}\right)^{-1}\underset{\sim}{\chi}'_{co} \\ \underset{\sim}{Z}'_{co} &= (it-1)\left(\underset{\sim}{\chi}'_{cc} - e^{-2\pi i\nu}\right)^{-1}\underset{\sim}{\chi}'_{co} \end{aligned}\right\} \qquad (4.43)$$

where

$$\underset{\sim}{\chi}'_{oc} = \underset{\sim}{\chi}_{oc}\,\underset{\sim}{X} \;,\; \underset{\sim}{\chi}'_{co} = \underset{\sim}{X}^T\underset{\sim}{\chi}_{co} \;,\; \underset{\sim}{Z}'_{co} = \underset{\sim}{X}^T\underset{\sim}{Z}_{co} \qquad (4.44)$$

From the unitarity of the $\underset{\sim}{\chi}$ matrix we get :

$$\underset{\sim}{X}^+\underset{\sim}{X} = \underset{\sim}{\chi}'^{*}_{co}\,\underset{\sim}{\chi}'_{oc} + \chi'^{*}_{cc}\,\underset{\sim}{X}^+\underset{\sim}{X}\,\chi'_{cc} \qquad (4.45)$$

with $\underset{\sim}{X}^+ = (\underset{\sim}{X}^T)^*$ ($*$: complex conjuguate)

Now if we write the eigenvalues of $\underset{\sim}{\chi}_{cc}$ as follow :

$$\chi'_{pp} = e^{2\pi i\mu_p} \tag{4.46}$$

where

$$\mu_p = \alpha_p + i\beta_p \tag{4.47}$$

we deduce from (4.45)

$$|\chi'_{pp}| \leq 1 \qquad \text{or} \qquad \beta_p \geq 0 \tag{4.48}$$

Seaton (1969) called μ_p the complex quantum defect.

If we denote the closed channels by p and q ,and the only open channel by 1 , we can write

$$Z_{p1} = (it-1)\sum_q \frac{X_{pq}\,\chi'_{q1}}{\chi'_{qq} - e^{-2\pi i\nu}} \tag{4.49}$$

The elements of $\underset{\sim}{X}$, $\underset{\sim}{\chi}'_{cc}$, $\underset{\sim}{\chi}'_{co}$ matrices vary slowly with energy.

Finally we obtain for Σ_{p1}

$$\Sigma_{p1} = i\sqrt{2\pi}\,\nu^{3/2} e^{-i\pi\nu} K_p \sum_q \frac{X_{pq}\,\chi'_{q1}}{\chi'_{qq} - e^{-2\pi i\nu}} \tag{4.50}$$

4-9 Bound states in the case of degenerate closed channels

We shall study the bound state case as the limiting case to which converges the open-closed channels problem when the interaction between open and closed channels is very small.

In this case χ_{cc} is unitary . From (4.45) we obtain

$$\chi'^{*}_{cc} = \chi'^{-1}_{cc}$$

that gives

$$|\chi'_{pp}| = 1 \qquad (4.51)$$

and also that $\underset{\sim}{\chi}$ is real

From Chapter II (2.31) we see that the bound states correspond to the energies when

$$\underset{\sim}{\Sigma}^{-1}_{cc} \underset{\sim}{M} = 0 \qquad (4.52)$$

From (4.39) we have

$$\underset{\sim}{\Sigma}^{-1}_{cc} = \frac{i}{\pi K \nu^{1/2}} \underset{\sim}{\chi} \left(e^{-2\pi i\nu} + \chi'_{cc} \right)^{-1} \left(e^{-2\pi i\nu} - \chi'_{cc} \right) \chi^{T} \frac{1}{K \nu^{3/2}} \qquad (4.53)$$

The bound states occur when

$$e^{-2\pi i\nu} = \chi'_{pp} \quad \left(= e^{2\pi i\alpha_p} \right)$$

i.e.

$$\nu = n - \alpha_p \qquad (4.54)$$

There is an infinite number of $\underset{\sim}{M}_{(p)}$ matrix satisfying (4.52) but in fact they are all linear dependant one of the other. One of them is :

$$\underset{\sim}{M}_{(p)} = \nu^{3/2} K \underset{\sim}{X}_{p} \tag{4.55}$$

$\underset{\sim}{X}_p$ is the column p extracted from $\underset{\sim}{X}$

Using a similar method to Seaton (1966) we can find a normalised solution $G^{N}_{(p)}(r)$:

$$\int G^{N\,+}_{(p)}(r)\, G^{N}_{(p)}(r)\, dr = 1 \tag{4.56}$$

by taking

$$\left.\begin{aligned} \underset{\sim}{M}_{(p)} &= K \underset{\sim}{X}_{p} \\ \underset{\sim}{G}^{N}_{(p)} &= -\phi^{+} \underset{\sim}{M}_{(p)} \end{aligned}\right\} \tag{4.57}$$

(We neglect the slowly variation of χ'_{pp} with energy. This approximation is valid for bound states having a large principal quantum number : for He^{+} + e^{-} $n \geq 4$)

4-10 Weak coupling between open and closed channels

When the interaction between open and closed channels is small the resonances are very narrow ($\beta_p \ll 1$) . The results obtained in 4-9 are true as a first order.

In the case of He^{+} + e^{-} the resonances are always narrow.

The $\underset{\sim}{X}$ matrix is nearly real :

$$\underset{\sim}{X}' = \underset{\sim}{X}^R + i\,\underset{\sim}{\delta X} \tag{4.58}$$

where $\underset{\sim}{X}^R$ and $\underset{\sim}{\delta X}$ are real matrices. We have

$$|\,\underset{\sim}{\delta X}\,| \ll 1 \tag{4.59}$$

Then it is easy to prove :

$$\left(X^+X\right)_{pp} = 1 + \left(2^{nd}\text{ order: } \delta X\,\delta X\right) \tag{4.60}$$

(diagonal element of X^+X)

From (4.45) we deduce

$$|\chi'_{p1}|^2 \simeq 1 - |\chi'_{pp}|^2 \tag{4.61}$$

and by consequence

$$|\chi'_{p1}|^2 \simeq 4\pi\beta_p \tag{4.62}$$

Another important point is that we can develop our resonance on "normalised bound states".

From (4.57) applied to (4.32),(4.50) we have

$$G_{q1}\left(\Sigma\,,r\right) \simeq i\sqrt{2\pi}\,\nu^{3/2}e^{-i\pi\nu}\sum_p \frac{G^N_{(p)q}\,\chi'_{p1}}{\chi'_{pp}-e^{-2\pi i\nu}} \tag{4.63}$$

where $G^N_{(p)q}$ is the element q of the column matrix $G^N_{(p)}$

i.e.

$$G^{N}_{(p)q} \sim e^{-\frac{r}{\nu}} \left(\frac{2r}{\nu}\right)^{\nu} K_q \, X^{R}_{qp} \qquad (4.64)$$

Let's come back to $\underset{\sim}{F}(\underset{\sim}{\mathcal{J}}, r)$ (Chapter II (2.27)), from 4-8 we have :

$$F_{q1}(\underset{\sim}{\mathcal{J}}, r) \simeq i\sqrt{2\pi}\, \nu^{3/2} e^{-i\pi\nu} \sum_{p} \frac{F^{N}_{(p)q}\, \chi'_{p1}}{\chi'_{pp} - e^{-2\pi i\nu}} \qquad (4.65)$$

where

$$F^{N}_{(p)q} \sim e^{-\frac{r}{\nu}} \left(\frac{2r}{\nu}\right)^{\nu} \sum_{r} O_{qr} \, K_r \, X^{R}_{rp} \qquad (4.66)$$

The matrix $\underset{\sim}{O}$ being orthogonal and real $F^{N}_{(p)}$ is a "normalised bound state" .

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CHAPTER V

Electron capture probability by photo-emission

In this chapter we use the Bates and Damgaard Approximation (1949) in order to enable us to utilise the results of Chapter IV in the interaction Hamiltonian, $\mathcal{H}_{\Gamma\Gamma'}(E)$, of Chapter III.

Hence, having a mathematical formula for $\mathcal{H}_{\Gamma\Gamma'}(E)$, we evaluate $\underset{\sim}{Z}(E)$ by two different methods. The two final results obtained for the capture probability differ by a term that is analysed .

5-1 Interaction Hamiltonian

The radiation field Hamiltonian was defined in Chapter III (3.10),(3.13) as

$$\mathcal{H}_{\Gamma\Gamma'}(E) = \left(\frac{2\omega^3\alpha^3}{3\pi}\right)^{1/2} \frac{1}{\sqrt{2\pi}} \frac{(\Gamma E \,\|\, \underset{\approx}{R} \,\|\, \Gamma')}{\sqrt{(2L+1)(2S+1)}} \qquad (5.1)$$

We shall do the following approximations :

1) We ignore the direct recombination $1sk\ell$ to $1sn\ell\pm1$ that is small in the resonances region for He$^+$ + e$^-$.

2) We neglect the second channel contribution ($2s\nu\ell$) since it gives only secondary effects .

3) The channels $2p\nu\ell+1$ and $2p\nu\ell-1$ recombine into the series of bound states $1sn'\ell+1$ and $1sn''\ell-1$ respectively .

4) The strong interaction between the 2p and 1s states of the core electron produces the photo-emission .

Due to the different core configurations (1s or 2p) the outer electron radial function $P^{(2p)}_{\nu\ell+1}$ with core 2p is different of any radial function $P^{(1s)}_{n'\ell+1}$ with core 1s (the same holds for $P^{(2p)}_{\nu\ell-1}$ and $P^{(1s)}_{n''\ell+1}$) . But if we suppose the radial functions $P^{(1s)}_{n'\ell+1}$ constitute a complete basis for the $P^{(2p)}_{\nu\ell+1}$ we have :

$$P^{(2p)}_{\nu\ell+1} = \sum_{n'} \mathcal{O}_{\nu\ell+1,n'\ell+1} \, P^{(1s)}_{n'\ell+1} \qquad (5.2)$$

with

$$\mathcal{O}_{\nu\ell+1,n'\ell+1} = \int_0^\infty P^{(2p)}_{\nu\ell+1} \, P^{(1s)}_{n'\ell+1} \, dr \qquad (5.3)$$

and

$$\sum_{n'} \left|\mathcal{O}_{\nu\ell+1,n'\ell+1}\right|^2 = 1 \qquad (5.4)$$

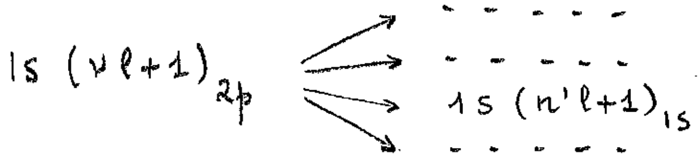
In practice $|\mathcal{O}_{\nu\ell,n\ell}|^2$ decreases rapidly when the difference $|\nu-n|^2$ increases.

Using this former decomposition we can simplify the problem by dividing the process in two parts

A - Photo-emission produced by the core electron

$$2p\,(\nu\,\ell+1)_{2p} \longrightarrow 1s\,(\nu\,\ell+1)_{2p} + \text{photon}$$

B - The outer electron recombines with a probability depending on the overlap integral .



This approximation will be valid only when the overlap integral will not spread over too many n' and also when ν will not be too small so that $\omega \simeq 1.5$ a.u.

In this chapter we shall only consider the part A : Each channel recombines into one "bound state" $1s\,(\nu\ell\pm1)_{2p}$. The Hamiltonian matrix defined in 3-3 contains 2 elements :

$$\underset{\sim}{\mathcal{H}}(E) = (\mathcal{H}_{11}\ ,\mathcal{H}_{12}) \tag{5.5}$$

$\mathcal{H}_{11}$ corresponds to : $2p\,(\nu\ell+1)_{2p} \longrightarrow 1s\,(\nu\ell+1)_{2p} + \text{photon}$
$\mathcal{H}_{12}$ corresponds to : $2p\,(\nu\ell-1)_{2p} \longrightarrow 1s\,(\nu\ell-1)_{2p} + \text{photon}$
Using Racah Algebra we obtain :

$$\left.\begin{aligned} \mathcal{H}_{11} &= \frac{1}{2\pi} A_r^{1/2} \int F^*_{31}(\underset{\sim}{\mathcal{E}}, r)\, P^{(2p)}_{\nu\,l+1}\, dr \\ \mathcal{H}_{12} &= \frac{1}{2\pi} A_r^{1/2} \int F^*_{41}(\underset{\sim}{\mathcal{E}}, r)\, P^{(2p)}_{\nu\,l-1}\, dr \end{aligned}\right\} \tag{5.6}$$

with

$$A_r = \frac{4}{3}\,\omega^3\alpha^3\,\frac{1}{3}\left|\int P_{2p}(r)\, r\, P_{1s}(r)\, dr\right|^2 \simeq 2.416\times10^{-7}\ \text{a.u.} \tag{5.7}$$

(P_{2p} and P_{1s} are the He^+ radial 2p and 1s functions)

5-2 Bates and Damgaard coulombic approximation

Before going further we shall justify the former decomposition using the Bates and Damgaard Approximation (1949) .

Let's consider the single channel radial equation . For $r = 0$ the bound channel solution $P_{\nu l}(r)$ satisfies the condition $P_{\nu l}(0) = 0$. For $r < r_0$, $P_{\nu l}(r)$ depends on the core considered and for $r \geqslant r_0$ the solution is known exactly for it is a coulombic function . Using a similar method to 4-9 we obtain for normalised bound solution :

$$P_{\nu l}(r) = K(\nu, l)\, e^{-\frac{r}{\nu}} \left(\frac{2r}{\nu}\right)^{\nu} \left\{ 1 + \sum_{t=1}^{\infty} \frac{a_t}{r^t} \right\} \qquad (5.8)$$

with

$$\left.\begin{aligned} a_1 &= \frac{\nu}{2} \Big(l(l+1) - \nu(\nu-1) \Big) \\ a_t &= a_{t-1} \left\{ \frac{\nu}{2t} \Big[l(l+1) - (\nu-t)(\nu-t+1) \Big] \right\} \end{aligned}\right\} \qquad (5.9)$$

In (5.8) we have introduced the full development of the coulombic solution (Whittaker function) .

When ν increases the radial function extends less and less into the core and by consequence its value out of the core contributes more and more in the interaction integrals (i.e. overlap, dipole ..... integrals) .

Bates and Damgaard Approximation is to use, for any r , (5.8) with a suitable cut-off to for the infinite sum . This cut-off has for purpose to suppress unwanted divergent terms in $\frac{1}{r^m}$. These terms are neglegible for r large . The choice of the cut-off can be varied but we prefered the one used by Burgess and Seaton (1960) for it looks more physical :

From (5.9) we see that for $\nu = n$ the series is finite $a_t = 0$ for $t \geq n-\ell$, for $t < n-\ell$ a_t is negative . For ν between $n-1$ and n the series is negative for $t < n-\ell$ and is positive for $t \geq n-\ell$. The smallest element in absolute value $|a_t|$ can be either for $t = n-\ell-1$ or $t = n-\ell$. Burgess and Seaton's choice for t_0 corresponds to this minimal element . We tried many different choices and we found the results are not very sensitive on the choice but the best results are obtained for Burgess and Seaton's choice (Our criteria was based on the computed normalisation obtained for different t_0) .

Bates and Damgaard Approximation is valid for the coupled equations if the coupling dissapears for $r \geq r_0$. For He$^+$ we applied B. & D. Approximation to the bound channels solutions for $\underset{\sim}{G}$ since the equations (5.8) and (5.9) are also valid for λ real or $\lambda = -\frac{1}{2} + i\bar{\lambda}$ (It is easy to check that for $\lambda = -\frac{1}{2} + i\bar{\lambda}$ the function $P_{\nu\lambda}(r)$ is real) . For these λ the definition of the cut-off t_0 can be generalised .

We require to compute

$$\theta_{\nu\lambda\,\nu'\lambda'} = \int_0^\infty P_{\nu\lambda}(r)\, P_{\nu'\lambda'}(r)\, dr \qquad (5.10)$$

On table 5*1,5*2,5*3 we give $\theta_{\nu\lambda\,\nu'\lambda'}$ for some values useful for L=0 and L=1 partial waves . On table 5*1 we consider $\lambda = \lambda'$ for ν and ν' varying from 12 to 13 . Due to the symmetry in ν and ν' we give only half of the table . We see that the results don't depend on λ . We did other computations for $|\nu - \nu'| \leq 4$ and it transpires from them that :

(1)

$\ell=0$	12.	12.2	12.4	12.6	12.8	13.
12.	1					
12.2	0.94	1				
12.4	0.76	0.94	1			
12.6	0.50	0.76	0.94	1		
12.8	0.23	0.50	0.76	0.94	1	
13.	0.	0.23	0.50	0.76	0.94	1

(2)

$\ell=1$	12.	12.2	12.4	12.6	12.8	13.
12.	1					
12.2	0.94	1.				
12.4	0.76	0.94	1.			
12.6	0.50	0.76	0.94	1.		
12.8	0.23	0.50	0.76	0.94	1.	
13.	0.	0.23	0.50	0.76	0.94	1.

(3)

$\ell=1.6$	12.	12.2	12.4	12.6	12.8	13.
12.	1.					
12.2	0.93	0.99				
12.4	0.75	0.92	0.99			
12.6	0.50	0.75	0.92	0.99		
12.8	0.22	0.50	0.75	0.92	0.99	
13.	-0.01	0.23	0.50	0.75	0.93	1.

(4)

$\ell=2$	12.	12.2	12.4	12.6	12.8	13.
12.	1.					
12.2	0.94	1.01				
12.4	0.76	0.95	1.03			
12.6	0.51	0.76	0.94	1.00		
12.8	0.23	0.51	0.76	0.94	1.00	
13.	0	0.23	0.50	0.76	0.94	1.

(5)

$\ell=2.137$	12.	12.2	12.4	12.6	12.8	13.
12.	0.98					
12.2	0.92	0.98				
12.4	0.74	0.92	0.99			
12.6	0.49	0.74	0.94	1.03		
12.8	0.23	0.50	0.75	0.93	0.98	
13.	0	0.23	0.50	0.75	0.92	0.98

(6)

$\ell=-\frac{1}{2}+0.999i$	12.	12.2	12.4	12.6	12.8	13.
12.	1.02					
12.2	0.95	1.01				
12.4	0.77	0.95	1.01			
12.6	0.51	0.76	0.95	1.02		
12.8	0.24	0.51	0.78	0.96	1.02	
13.	0	0.24	0.52	0.77	0.95	1.02

TABLE 5*1

(1)

ℓ=1 ℓ=0	12.	12.2	12.4	12.6	12.8	13.
12.	1.	0.96	0.80	0.55	0.28	0.03
12.2	0.91	1.	0.96	0.80	0.55	0.28
12.4	0.71	0.91	1.	0.96	0.80	0.55
12.6	0.46	0.72	0.91	1.	0.96	0.79
12.8	0.19	0.46	0.72	0.91	1.	0.96
13.	-0.02	0.20	0.46	0.72	0.91	1.

(2)

ℓ=1 ℓ=0	8.	8.2	8.4	8.6	8.8	9.0
8.	0.99	0.96	0.81	0.57	0.29	0.05
8.2	0.89	0.99	0.96	0.80	0.57	0.30
8.4	0.69	0.89	0.99	0.95	0.81	0.57
8.6	0.44	0.69	0.89	0.99	0.96	0.81
8.8	0.18	0.44	0.70	0.90	0.99	0.96
9.	-0.03	0.18	0.44	0.70	0.90	0.99

(3)

ℓ=2 ℓ=1	12.	12.2	12.4	12.6	12.8	13.
12.	0.99	0.97	0.83	0.60	0.32	0.06
12.2	0.88	0.99	0.97	0.83	0.60	0.32
12.4	0.67	0.87	0.98	0.97	0.83	0.60
12.6	0.41	0.67	0.88	0.99	0.97	0.83
12.8	0.16	0.41	0.67	0.88	0.99	0.97
13.	-0.04	0.16	0.42	0.67	0.88	0.99

(4)

ℓ=2 ℓ=0	12.	12.2	12.4	12.6	12.8	13.
12.	0.97	0.98	0.86	0.64	0.37	0.10
12.2	0.84	0.97	0.98	0.86	0.64	0.37
12.4	0.63	0.85	0.97	0.98	0.86	0.64
12.6	0.37	0.63	0.85	0.97	0.98	0.86
12.8	0.13	0.37	0.63	0.85	0.98	0.98
13.	-0.06	0.13	0.38	0.63	0.85	0.98

(5)

ℓ=1.6 ℓ=0	12.	12.2	12.4	12.6	12.8	13.
12.	0.98	0.96	0.83	0.59	0.32	0.06
12.2	0.87	0.98	0.96	0.82	0.59	0.32
12.4	0.67	0.87	0.98	0.96	0.82	0.59
12.6	0.41	0.67	0.87	0.98	0.96	0.82
12.8	0.16	0.41	0.67	0.88	0.98	0.96
13.	-0.04	0.16	0.41	0.67	0.88	0.98

(6)

ℓ=2.237 ℓ=0	12.	12.2	12.4	12.6	12.8	13.
12.	0.95	0.97	0.87	0.66	0.39	0.12
12.2	0.82	0.95	0.97	0.87	0.66	0.39
12.4	0.60	0.82	0.96	0.97	0.86	0.65
12.6	0.35	0.60	0.82	0.96	0.97	0.86
12.8	0.11	0.35	0.61	0.82	0.96	0.97
13.	-0.06	0.12	0.35	0.61	0.83	0.96

TABLE 5*2

(1)

$\ell=1.6$ $\ell=1$	12.	12.2	12.4	12.6	12.8	13.
12.	0.99	0.95	0.79	0.55	0.28	0.03
12.2	0.90	0.99	0.95	0.79	0.55	0.28
12.4	0.70	0.90	0.99	0.95	0.79	0.55
12.6	0.45	0.71	0.90	0.99	0.95	0.79
12.8	0.19	0.46	0.71	0.90	0.99	0.95
13.	-0.02	0.19	0.46	0.71	0.90	0.99

(2)

$\ell=2.237$ $\ell=1$	12.	12.2	12.4	12.6	12.8	13.
12.	0.97	0.97	0.84	0.62	0.34	0.08
12.2	0.85	0.97	0.96	0.84	0.61	0.34
12.4	0.64	0.85	0.97	0.96	0.84	0.61
12.6	0.39	0.64	0.85	0.97	0.97	0.84
12.8	0.14	0.39	0.64	0.85	0.97	0.97
13.	-0.05	0.14	0.39	0.65	0.86	0.97

(3)

$\ell=2.237$ $\ell=2$	12.	12.2	12.4	12.6	12.8	13.
12.	0.99	0.94	0.77	0.52	0.25	0.01
12.2	0.91	0.99	0.95	0.79	0.53	0.26
12.4	0.72	0.91	1.	0.97	0.78	0.53
12.6	0.47	0.73	0.92	1.	0.94	0.77
12.8	0.21	0.48	0.73	0.92	0.99	0.94
13.	-0.01	0.21	0.48	0.73	0.91	0.99

(4)

$\ell=-\frac{1}{2}+i0.999$ $\ell=0$	12.	12.2	12.4	12.6	12.8	13.
12.	1.	0.93	0.74	0.49	0.22	-0.01
12.2	0.96	1.	0.93	0.74	0.49	0.22
12.4	0.78	0.96	1.	0.93	0.74	0.49
12.6	0.53	0.78	0.96	1.	0.93	0.74
12.8	0.26	0.53	0.78	0.96	1.	0.93
13.	0.01	0.26	0.53	0.78	0.95	1.

(5)

$\ell=-\frac{1}{2}+i0.999$ $\ell=1$	12.	12.2	12.4	12.6	12.8	13.
12.	1.	0.90	0.70	0.44	0.18	-0.03
12.2	0.97	1.	0.90	0.70	0.44	0.18
12.4	0.82	0.97	1.	0.90	0.70	0.44
12.6	0.58	0.82	0.97	1.	0.91	0.70
12.8	0.30	0.58	0.82	0.97	1.	0.91
13.	0.05	0.30	0.58	0.82	0.97	1.

(6)

$\ell=-\frac{1}{2}+i0.999$ $\ell=2$	12.	12.2	12.4	12.6	12.8	13.
12.	0.97	0.84	0.61	0.36	0.12	-0.06
12.2	0.99	0.97	0.84	0.62	0.36	0.12
12.4	0.88	0.99	0.98	0.84	0.62	0.36
12.6	0.67	0.88	0.99	0.98	0.84	0.62
12.8	0.40	0.67	0.88	0.99	0.98	0.84
13.	0.12	0.39	0.67	0.88	0.99	0.98

TABLE 5*3

$$\vartheta_{\nu\lambda\,\nu'\lambda} = \frac{\sin\pi(\nu-\nu')}{\pi(\nu-\nu')} \qquad (5.11)$$

(5.11) agrees with (5.4) since it can be proved (Cartan (1963)) that :

$$\sum_{n=-\infty}^{+\infty} \frac{1}{(x-n)^2} = \left(\frac{\pi}{\sin\pi x}\right)^2 \qquad (5.12)$$

On table 5*2 and 5*3 we give results for $\lambda \neq \lambda'$ which are slightly asymmetrical but if we compare 5*2 (1) and (2) that correspond to $\lambda = 0$ and $\lambda = 1$ for ν , ν' between 12 and 13 and ν , ν' between 8 and 9 we see that the asymmetry dissapears when ν increases . For ν large we can deduce at the first order that

$$\vartheta_{\nu\lambda\,\nu'\lambda'} \simeq \frac{\sin\pi(\nu-\nu')}{\pi(\nu-\nu')} \qquad (5.13)$$

Applying (5.13) in (5.6) and using (4.65) we obtain :

$$\left.\begin{aligned} \mathcal{H}_{11} &= -\frac{i}{\sqrt{2\pi}} A_r^{\frac{1}{2}} \nu^{\frac{3}{2}} e^{i\pi\nu} \sum_t O_{3t} \sum_p \frac{X^*_{tp} \chi'^*_{p1}}{\chi'^*_{pp} - e^{2\pi i\nu}} \\ \mathcal{H}_{12} &= -\frac{i}{\sqrt{2\pi}} A_r^{\frac{1}{2}} \nu^{\frac{3}{2}} e^{i\pi\nu} \sum_t O_{4t} \sum_p \frac{X^*_{tp} \chi'^*_{p1}}{\chi'^*_{pp} - e^{2\pi i\nu}} \end{aligned}\right\} \qquad (5.14)$$

For calculating the $\underset{\sim}{S}^{(p,e)}$ matrix we need to know the $\underset{\sim}{Z}$ matrix . In the next parts we shall give two different methods for evaluating $\underset{\sim}{Z}$ (and $\underset{\sim}{S}^{(p,e)}$) .

5-3 Energy representation

Due to an existing phase difference we shall consider only the case where the resonances do not overlap .

The resonances being very narrow we can do an energy expansion of $(\chi'_{pp} - e^{-2\pi i\nu})$ around each resonance center $\nu_{np} = n - \alpha_p$.

$$\chi'_{pp} - e^{-2\pi i\nu} = e^{2\pi i\alpha_p}\left(e^{-2\pi\beta_p} - e^{-2\pi i\delta\nu}\right) \qquad (5.15)$$

where

$$\left.\begin{aligned} \delta\nu &= \nu - \nu_{np} \simeq \nu_{np}^3\,(E - E_{np}) \\ E_{np} &= E_{2p}^{+} - \frac{1}{2\nu_{np}^2} \end{aligned}\right\} \qquad (5.16)$$

E_{2p}^{+} is the excitation energy from 1s to 2p , $E_{2p}^{+} = 1.5$ a.u

We shall also define

$$\Gamma_{np} = \frac{2\beta_p}{\nu_{np}^3} \qquad (5.17)$$

At the first order (5.15) is

$$\chi'_{pp} - e^{-2\pi i\nu} \simeq 2\pi i\,\nu_{np}^3\, e^{2\pi i\alpha_p}\left(E - E_{np} + i\,\frac{\Gamma_{np}}{2}\right) \qquad (5.18)$$

The resonances don't overlap and the coupling between open and closed channels being weak we can deduce

near $\nu = \nu_{np}$

$$\left(\underset{\sim}{\mathcal{H}}^{+}\underset{\sim}{\mathcal{H}}\right)_{ij} = \frac{1}{4\pi^2}\, A_r \sum_{ts} O_{i't}\, O_{j's}\, \frac{X_{tp}X^{*}_{sp}\,\Gamma_{np}}{(E - E_{np})^2 + \frac{1}{4}\Gamma_{np}^2} \qquad (5.19)$$

i' and j' are defined as follow :

$$\left.\begin{array}{l} i=1 \longleftrightarrow i'=3 \\ i=2 \longleftrightarrow i'=4 \end{array}\right\} \quad \text{the same for } j \text{ and } j'$$

From the Residue theorem we have :

$$\underset{\sim}{Z}(E) = \frac{i}{2} A_r \sum_{ts} O_{i't} O_{j's} \frac{X_{tp} X^*_{sp}}{(E-E_{np}) + \frac{i}{2}\Gamma_{np}} \qquad (5.20)$$

we define the column matrix (2,1) $\underset{\sim}{B}_p$ by

$$\underset{\sim}{B}_p = A_r^{1/2} \underset{\sim}{O}' \underset{\sim}{X}_p \qquad (5.21)$$

where

$$\underset{\sim}{O}' = \begin{pmatrix} O_{32} & O_{33} & O_{34} \\ O_{42} & O_{43} & O_{44} \end{pmatrix} \qquad (5.22)$$

$\underset{\sim}{X}_p$ is the column number p of $\underset{\sim}{X}$

$$\underset{\sim}{Z}(E) = \frac{i}{2} \frac{1}{E-E_{np}+\frac{i}{2}\Gamma_{np}} \underset{\sim}{B}_p \underset{\sim}{B}^+_p \qquad (5.23)$$

Then

$$\underset{\sim}{S}^{(p,e)} = e^{i\varphi}\left(E-E_{np}+\frac{i}{2}\Gamma_{np}+\frac{i}{2}\underset{\sim}{B}_p\underset{\sim}{B}^+_p\right)^{-1}\underset{\sim}{B}_p\Gamma_{np} \qquad (5.24)$$

(φ is a phase depending on $\arg(\chi'_{pp})$ and $\arg(\chi'_{p1})$)

The right hand side of (5.24) contains a matrix (2,2) to inverse . The formulation is simplify by using the following formula :

$$\left(1+\underset{\sim}{B}\,\underset{\sim}{A}\,\underset{\sim}{B}^{+}\right)^{-1}\underset{\sim}{B} \equiv \underset{\sim}{B}\left(1+\underset{\sim}{A}\,\underset{\sim}{B}^{+}\underset{\sim}{B}\right)^{-1} \qquad (5.25)$$

very easy to prove since

$$\left(1+\underset{\sim}{B}\,\underset{\sim}{A}\,\underset{\sim}{B}^{+}\right)^{-1}\left(1+\underset{\sim}{B}\,\underset{\sim}{A}\,\underset{\sim}{B}^{+}\right)\underset{\sim}{B} \equiv \underset{\sim}{B} \qquad (5.26)$$

$$\left(1+\underset{\sim}{B}\,\underset{\sim}{A}\,\underset{\sim}{B}^{+}\right)^{-1}\underset{\sim}{B}\left(1+\underset{\sim}{A}\,\underset{\sim}{B}^{+}\underset{\sim}{B}\right) \equiv \underset{\sim}{B} \qquad (5.27)$$

This gives (5.25) by multiplying (5.27) by $\left(1+\underset{\sim}{A}\,\underset{\sim}{B}^{+}\underset{\sim}{B}\right)^{-1}$.

We have

$$\underset{\sim}{S}^{(p,e)} = e^{i\varphi}\,\Gamma_{np}\,\underset{\sim}{B}_p\left(E-E_{np}+\frac{i}{2}\Gamma_{np}+\frac{i}{2}\underset{\sim}{B}_p^{+}\underset{\sim}{B}_p\right)^{-1} \qquad (5.28)$$

$\underset{\sim}{B}_p^{+}\underset{\sim}{B}_p$ is a single element matrix .

$$\underset{\sim}{B}_p^{+}\underset{\sim}{B}_p \equiv A_r\left[\left|O_{32}X_{1p}+O_{33}X_{2p}+O_{34}X_{3p}\right|^2+\left|O_{42}X_{1p}+O_{43}X_{2p}+O_{44}X_{3p}\right|^2\right] \qquad (5.29)$$

The total recombination probability is

$$\underset{\sim}{S}^{(p,e)}+\underset{\sim}{S}^{(pe)} = \frac{\underset{\sim}{B}_p^{+}\,\underset{\sim}{B}_p\,\Gamma_{np}}{\left|E-E_{np}+\frac{i}{2}\Gamma_{np}+\frac{i}{2}\underset{\sim}{B}_p^{+}\underset{\sim}{B}_p\right|^2} \qquad (5.30)$$

and if we integrate over the resonance we obtain the probability to recombine into the resonance ν_{np} .

$$P(np) = \int dE\, S^{(p,e)+} S^{(p,e)}$$

$$= \frac{2\pi\, \underset{\sim}{B}_p^{+} \underset{\sim}{B}_p\, \Gamma_{np}}{\Gamma_{np} + \underset{\sim}{B}_p^{+} \underset{\sim}{B}_p} \qquad (5.31)$$

The formula (5.31) is very similar to the one obtained by Bates and Dalgarno (1962) .

5-4 Principal quantum number representation

In 5-3 we developed $\mathcal{H}_{1i}$ in function of the energy now we develop $\frac{1}{E-\Omega-i\epsilon}$, in formula (3.30) , in function of ν . The integral from $-\infty$ to $+\infty$, for E , is from ν_0 to ν_0+1 .

Using the same method introduced in 5-3 we expand E around $\Omega + i\epsilon$

$$E - \Omega - i\epsilon \simeq \frac{1}{\nu_\Omega^3} (\nu - \nu_\Omega - i \xi) \qquad (5.32)$$

with

$$\Omega = E^{+}_{2p} - \frac{1}{2\nu_\Omega^2} \quad , \quad E - \Omega = \frac{\nu - \nu_\Omega}{\nu_\Omega^3} \qquad (5.33)$$

and

$$i\epsilon = \frac{i\,\xi}{\nu_\Omega^3} \qquad (5.34)$$

with $\xi > 0$ (since $\epsilon > 0$)

Let's define

$$\chi_{\Omega\xi} = e^{2\pi i(\nu_\Omega + i\xi)} \qquad (5.35)$$

Then from (5.32) we obtain

$$\frac{1}{E-\Omega-i\epsilon} \simeq \frac{2\pi i\,\nu^3\,\chi_{\Omega\xi}}{e^{2\pi i\nu} - \chi_{\Omega\xi}} \qquad (5.36)$$

We can check this formula knowing that the integral of the left hand side of (5.36) is

$$\lim_{\epsilon\to 0}\int\frac{dE}{E-\Omega-i\epsilon} = i\pi \qquad (5.37)$$

for the right hand side it gives

$$\int_{\nu_0}^{\nu_0+1}\frac{d\nu}{\nu^3}\,\frac{2\pi i\,\nu^3\,\chi_{\Omega\xi}}{e^{2\pi i\nu}-\chi_{\Omega\xi}} = \oint\frac{dz\,\chi_{\Omega\xi}}{z(z-\chi_{\Omega\xi})} = 0 \qquad (5.38)$$

Therefore (5.36) is not correct .

We shall improve (5.36) using the approximation $\chi_{\Omega\xi} \simeq e^{2\pi i\nu}$ when $\nu \simeq \nu_\Omega$ and we can take :

$$\frac{1}{E-\Omega-i\epsilon} \simeq \frac{\pi i\,\nu^3\,(e^{2\pi i\nu} + \chi_{\Omega\xi})}{e^{2\pi i\nu} - \chi_{\Omega\xi}} \qquad (5.39)$$

This formula agrees with (5.37) . Also the right hand side is antisymmetrical in $e^{2\pi i\nu}$ and $\chi_{\Omega\xi}$ as the left hand side in E and $\Omega + i\epsilon$.

We write $\underset{\sim}{\mathcal{H}}^{+}(E)$ using the matrix notation

$$\underset{\sim}{\mathcal{H}}^{+}(E) = \frac{i}{\sqrt{2\pi}}\,\nu^{3/2} e^{-i\pi\nu}\,\underset{\sim}{B}\left(\chi'_{cc} - e^{-2\pi i\nu}\right)^{-1}\underset{\sim}{\chi}'_{co} \qquad (5.40)$$

$\underset{\sim}{B}$ is given by

$$\underset{\sim}{B} = A_r^{1/2}\,\underset{\sim}{O}'\,\underset{\sim}{X} \qquad (5.41)$$

If we compare (5.41) and (5.21) we see that $\underset{\sim}{B}_p$ is the column number p of $\underset{\sim}{B}$. $\underset{\sim}{B}$ is a (2,3)-matrix .

Using (5.39) we have

$$\underset{\sim}{Z}(E) = \frac{\pi}{2}\,\nu^{3}\,\underset{\sim}{B}\left(e^{-2\pi i\nu} - \chi'_{cc}\right)^{-1}\left(e^{-2\pi i\nu} + \chi'_{cc}\right)\underset{\sim}{B}^{T} \qquad (5.42)$$

Applying (4.45) to (5.42) we reobtain (3.37) i.e. :

$$\underset{\sim}{Z}(E) + \underset{\sim}{Z}^{+}(E) = 2\pi^{2}\,\underset{\sim}{\mathcal{H}}^{+}\underset{\sim}{\mathcal{H}}$$

This is another check that (5.39) is correct .

The next stage is to reduce :

$$\underset{\sim}{S}^{(p,e)} = -\sqrt{2\pi}\,e^{-i\pi\nu}\,\nu^{3/2}\left(1 + \frac{\pi}{2}\nu^{3}\underset{\sim}{B}\left(e^{-2\pi i\nu} - \chi'_{cc}\right)^{-1}\left(e^{-2\pi i\nu} + \chi'_{cc}\right)\underset{\sim}{B}^{T}\right)^{-1}\underset{\sim}{B}\left(\chi'_{cc} - e^{-2\pi i\nu}\right)^{-1}\underset{\sim}{\chi}'_{co} \qquad (5.43)$$

by incorporating (5.25) and defining

$$\Delta_{cc} = \frac{\pi}{2}\,\nu^{3}\,\underset{\sim}{B}^{T}\underset{\sim}{B} \qquad (5.44)$$

We have

$$\underset{\sim}{S}^{(p,c)} = \sqrt{2\pi}\, e^{-i\pi\nu}\, \nu^{3/2}\, \underset{\sim}{B} \left(e^{-2\pi i\nu} - \underset{\sim}{\Theta}_{cc} \right)^{-1} \left(1 + \underset{\sim}{\Delta}_{cc} \right)^{-1} \underset{\sim}{\chi}'_{co} \qquad (5.45)$$

where

$$\Theta_{cc} = \left(1 + \underset{\sim}{\Delta}_{cc} \right)^{-1} \underset{\sim}{\chi}'_{cc} \left(1 - \underset{\sim}{\Delta}_{cc} \right) \qquad (5.46)$$

In general Θ_{cc} has not the same eigenvalues as χ'_{cc} . The matrix $\underset{\sim}{\Delta}_{cc}$ produces a shift in the positions of the resonances.

For comparing this new result to the former one (5.28) we shall do the same hypothesis : i.e. the resonances don't overlap .

For ν around ν_{np} :

$$\underset{\sim}{H}^{+} \underset{\sim}{H} = \frac{1}{4\pi^2}\, \underset{\sim}{B}_p \underset{\sim}{B}_p^{+} \frac{|\chi'_{p1}|^2}{(\chi'^{*}_{pp} - e^{2\pi i\nu})(\chi'_{pp} - e^{-2\pi i\nu})} \qquad (5.47)$$

Then

$$\underset{\sim}{Z}(E) = \frac{\pi}{2}\, \nu^3\, \underset{\sim}{B}_p \underset{\sim}{B}_p^{+} \frac{(e^{-2\pi i\nu} + \chi'_{pp})}{(e^{-2\pi i\nu} - \chi'_{pp})} \qquad (5.48)$$

and

$$\underset{\sim}{S}^{(p,e)} = \sqrt{2\pi}\, e^{-i\pi\nu}\, \nu^{3/2}\, \underset{\sim}{B}_p \left(e^{-2\pi i\nu} - \theta'_p \right)^{-1} \left(1 + \Delta'_p \right)^{-1} \chi'_{p1} \tag{5.49}$$

where

$$\Delta'_p = \frac{\pi}{2}\, \nu^3\, \underset{\sim}{B}_p^{\dagger} \underset{\sim}{B}_p \tag{5.50}$$

Δ'_p is a single element matrix as Θ'_p :

$$\Theta'_p = \left(1 + \Delta'_p \right)^{-1} \chi'_{pp} \left(1 - \Delta'_p \right) \tag{5.51}$$

Now using (4.61) we obtain

$$P(np) = \frac{2\pi\, |\chi'_{p1}|^2\, \underset{\sim}{B}_p^{\dagger} \underset{\sim}{B}_p}{2\pi \nu^3 \underset{\sim}{B}_p^{\dagger} \underset{\sim}{B}_p + |\chi'_{p1}|^2 \left(1 - \frac{\pi}{2} \nu^3 \underset{\sim}{B}_p^{\dagger} \underset{\sim}{B}_p \right)^2} \tag{5.52}$$

Inserting (4.62) and (5.17) the final result is deduced

$$P(np) = \frac{2\pi\, \underset{\sim}{B}_p^{\dagger} \underset{\sim}{B}_p}{\underset{\sim}{B}_p^{\dagger} \underset{\sim}{B}_p + \Gamma_{np} \left(1 - \frac{\pi}{2} \nu^3 \underset{\sim}{B}_p^{\dagger} \underset{\sim}{B}_p \right)^2} \tag{5.53}$$

If we compare (5.53) and (5.31) we see that they are identical except for the term $-\frac{\pi}{2} \nu^3 \underset{\sim}{B}_p^{\dagger} \underset{\sim}{B}_p$.

5-5 Commentary on the formulae obtained

The problem is to choose between (5.31) and (5.53) .

If we consider the case where the resonances are flat ($|\chi'_{p_1}|^2 = 1$) and do an average integration over ν we obtain from (5.31) :

$$< | S^{(p,e)\dagger} S^{(p,e)} | >^{(1)} = \frac{2\pi\nu^3 \underset{\sim}{B}_p^\dagger \underset{\sim}{B}_p}{1 + 2\pi\nu^3 \underset{\sim}{B}_p^\dagger \underset{\sim}{B}_p} \qquad (5.54)$$

Now let's do the same for (5.53)

$$< | S^{(p,e)\dagger} S^{(p,e)} | >^{(2)} = \frac{2\pi\nu^3 \underset{\sim}{B}_p^\dagger \underset{\sim}{B}_p}{\left(1 + \frac{\pi}{2}\nu^3 \underset{\sim}{B}_p^\dagger \underset{\sim}{B}_p\right)^2} \qquad (5.55)$$

When the resonances are flat there is no damping due to the resonances and we can compare the formulae (5.54) and (5.55) to the case where there is no resonance (Davies and Seaton formula (6,16))

$$S^{(p,e)\dagger} S^{(p,e)} = \frac{2\pi\,\Gamma(E)}{\left(1 + \frac{\pi}{2}\,\Gamma(E)\right)^2} \qquad (5.56)$$

where

$$\Gamma(E) = 2\pi\,\mathcal{H}^{+}(E)\,\mathcal{H}(E) \qquad (5.57)$$

We can therefore deduce that (5.53) is a better approximation than (5.31) .

For dielectronic recombination, the effect of using (5.53) instead of (5.31) appears for ν large. For $He^+ + e^-$ this effect is negligible since it appears for $\nu^3 \geqslant 10^7$ and at this point the dielectronic recombination is already small . But for more ionised system it can decrease considerably the dielectronic recombination rate .

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CHAPTER VI

Calculation of the complex quantum defect for $He^+ + e^-$

6-1 Introduction

In chapter V the electron capture probability was expressed in function of two quantities Γ_{np} and $\underset{\sim}{B}_p$ which were themselves function of the complex quantum defect ν_p and of the diagonalisation matrices $\underset{\sim}{O}$ and $\underset{\sim}{X}$. All these last quantities are tabulated in this chapter . They are obtained by a computation method deduced from chapter IV theory.

In this chapter we also check the validity of the method used by comparing the complex quantum defect to the values obtained by solving directly the coupled equations, employing the method developped by Norcross and Seaton (1970) . For completing the test we also built a programme using Bely's method (1965 a,b and 1966) .

We shall begin by giving some commentaries on this last test .

6-2 Bely's programme

Before developping chapter IV theory we thought possible to use Norcross and Seaton' method (1970) so as to extrapolate the complex quantum defect. But as will be shown in 6-4 (Figures 6*1 to 6*5) with this approximation any extrapolation of the complex quantum defect from above the threshold is unreliable. But on figures 6*1 to 6*5 an interesting feature appears : under the threshold the complex quantum defect is slowly varying with energy and seems to converge to the value obtained at the threshold. However we can't have any certainty since just under the threshold an unknown gap can't be reached by solving numerically the coupled equations.

We built Bely's programme (1965 a,b and 1966) to check, for $He^+ + e^-$, that the failure of Norcross and Seaton's method was really due to the difference of approximation. The direct comparaison of the asymptotic forms obtained by solving the coupled equations and the corresponding results deduced by extrapolation from above the threshold using Bely's programme was very good, showing a great improvement.

However Bely's programme didn't solve our problem :
First, it didn't give the complex quantum defect.
Second, it didn't fill the unknown gap due to some divergent functions used by the method.
Third, it was numerically very unstable depending on the computer word length. This point was already mentionned by Bely (1966) : " The calculations are very sensitive to numerical inaccuracies ".

For going out of this cul de sac we tried to improve Bely's method so as to suppress the divergent functions and the causes of the inaccuracies. We found that for some λ the analytic functions y_1, y_2 (and y_6, y_7 in Bely's notations) were not numerically independant when the word length was small . We defined new analytic functions giving less trouble . At the place of y_2 we took

$$y_2' = \frac{1}{2\pi} \left\{ A(\kappa, \ell)\, y_1 + y_2 \right\} / (\lambda - \ell)$$

that converged to y_4 for λ tending to an integer . These new functions improved the stability but increased the complexity of the programme already difficult to utilise . Also the number of possible new definitions being infinite the physical validity of any choice became problematical . We had to find a criteria .

Following Eissner et al. (1969) Seaton (1969 a) and Norcross and Seaton (1970) we decided to abandon the analytic functions for the slowly varying functions . For $\lambda = \ell$ the regular and irregular Coulomb function are slowly varying with energy . They are also in phase quadrature and they have physical properties in the Coulomb-Born Approximation . For $\lambda \neq \ell$ s° and c° are the natural prolongation of the Coulomb function .

Bely's programme has been kept for comparaison .

6-3 Chapter IV theory programme

For avoiding to compute many times the same quantities we built two programmes (for IBM 360) .

Programme I

INPUT : all the total angular momenta L corresponding to the partial waves considered (in practice : $L = 0, ----, 10$)

MAIN : reads the input and calls two subroutines AMAT , EIGEN . It prints and punchs the a and $\underset{\sim}{O}$ (see (4.6))

AMAT : from the target radial functions and the angular momenta L it calculates $\underset{\sim}{A}$ defined by (4.5) . For $He^+ + e^-$ we have

$$A = \begin{pmatrix} \ell_1(\ell_1+1) & 0 & 0 & 0 \\ 0 & \ell_1(\ell_1+1) & \frac{3\sqrt{\ell_1+1}}{\sqrt{2\ell_1+1}} & \frac{-3\sqrt{\ell_1}}{\sqrt{2\ell_1+1}} \\ 0 & \frac{3\sqrt{\ell_1+1}}{\sqrt{2\ell_1+1}} & (\ell_1+1)(\ell_1+2) & 0 \\ 0 & \frac{-3\sqrt{\ell_1}}{\sqrt{2\ell_1+1}} & 0 & \ell_1(\ell_1-1) \end{pmatrix} \qquad (6.1)$$

EIGEN : it calculates the diagonal matrix a and the orthogonal matrix O ($a_{11} = A_{11}$ and $O_{i1} = 0$ excepted $O_{11} = 1$) . EIGEN is derived from CEIGEN (see Programme II) .

Programme II

INPUT :

a : L , a , $\underset{\sim}{O}$

b : number of energies from which the extrapolation is done : $N1$, and number of energies to which the extrapolated results will be calculated : $N2$.

c : energies corresponding to $N1$ and $N2$: $E1(i)$, $E2(j)$

d : $\underset{\sim}{R}$ matrices obtained from the coupled equations programme and corresponding to : L , $E1(i)$

e : degree of the polymonial fitting + 1 : N . If the value is zero the programm takes $N = N1$.

MAIN : the inputs are read and the four main subroutine are called : RTORP , ANALYT , RPTOR , RESON .

RTORP : it does the transformation from $\underset{\sim}{R}$ to $\underset{\sim}{\mathcal{R}}$. The elements required for this transformation are computed in PHI .

ANALYT : knowing the $\underset{\sim}{\mathcal{R}}$ -matrices corresponding to L , $E1(i)$ it obtains the coefficient matrices of the polymonial expansion of degree $N-1$.

$$\underset{\sim}{\mathcal{R}} = \underset{\sim}{\mathcal{R}}_1 + \underset{\sim}{\mathcal{R}}_2 E + ---- \underset{\sim}{\mathcal{R}}_N E^{N-1} \qquad (6.2)$$

Depending on $\mathcal{N}$ the subroutine uses different methods :
For $\mathcal{N} = N1$ it uses the direct fitting obtained by inversing the matrix

$$\underset{\sim}{D} = \begin{pmatrix} 1 & E_1 & E_1^2 & \cdots & E_1^{N1-1} \\ 1 & E_2 & E_2^2 & \cdots & E_2^{N1-1} \\ - & - & - & - & - \\ - & - & - & - & - \\ 1 & E_{N1} & E_{N1}^2 & & E_{N1}^{N1-1} \end{pmatrix} \qquad (6.3)$$

For $N < N1$ it uses the least square polymonial fitting ($1 \leqslant N < N1$) . The problem reduces to a matrix inversion as in the first case . For $N = N1$ the second method is identical to the first . The subroutine calls INV .

RPTOR : from the matrices $\underset{\sim}{\mathcal{R}}_1$, ... ,$\underset{\sim}{\mathcal{R}}_N$ it rebuilts the $\underset{\sim}{\mathcal{R}}$ -matrix for the required energy . Then by calling PHI it transforms $\underset{\sim}{\mathcal{R}}$ into $\underset{\sim}{R}$ or $\underset{\sim}{\mathscr{R}}$ (see (2.26)) it prints the matrix obtained .

RESON : it obtains from the $\underset{\sim}{\mathcal{R}}$ matrix the resonance structure matrices $\underset{\sim}{\mathcal{X}}_{cc}$, $\mathcal{X}'_{cc}$ and $\underset{\sim}{X}$. For diagonalising $\mathcal{X}_{cc}$ the programme calls CEIGEN .All the quantities obtained are print included the $\underset{\sim}{\Omega}$ matrix defined by : $\Omega_{i\gamma} = |(\underset{\sim}{Q}\,\underset{\sim}{X})_{i\gamma}|^2$.
The complex quantum defect $\mu_p = \mathcal{X}'_{pp}$ and the elements $\Omega_{i\gamma}$ are tabulated on table 6*6 to 6*25 .

PHI : knowing a and E it deduces λ ($a_{ii} = \lambda_i(\lambda_i+1)$) and the

ϵ_i for each,channel . Then for $\epsilon_i \geq 0$ from (2.17) (4.23) (4.24) and (4.27) it obtains the two phases differences that are necessary for doing the transformation from $\underset{\sim}{R}$ to $\underset{\sim}{\mathcal{A}}$ (and vice-versa) (see Appendix 3) . For $\epsilon_i < 0$ from (4.20) it obtains the expansion coefficients on the convergent and divergent asymptotic functions (by eliminating the divergent part $\underset{\sim}{\mathcal{R}}$ is deduced in RPTOR). PHI calls GAMC .

GAMC : it gives the modulus and argument of $\Gamma(z)$ when z is complex . The method used is classical : for $\mathcal{R}e(z) < 10$ it uses the canonical relation $\Gamma(z) = z\,\Gamma(z-1)$ so that to express $\Gamma(z)$ in function of $\Gamma(z+n)$ where $\mathcal{R}e(z+n) \geq 10$. Then $\Gamma(z+n)$ is evaluated by the Stirling formula :

$$\Gamma(x) = e^{-x}\, x^{x-\frac{1}{2}}\, (2\pi)^{1/2} \left[1 + \frac{1}{12x} + \frac{1}{288x^2} - \frac{139}{51840x^3} - \frac{571}{2488320x^4} + \cdots \right] \qquad (6.4)$$

We checked GAMC by reprducing all the tables given by Abramowitz and Stegun (1965) . The agreement is over all the tabulated digits We also checked many other cases using for comparaison the formula

$$\Gamma(x)\;\Gamma(1-x) = \frac{\pi}{\sin(\pi x)} \qquad (6.5)$$

The agreement was very good .

CEIGEN : This programme was made by Seaton (1969 b) . It is a programme of diagonalisation of symmetric complex matrix .

INV : classical programme of matrix inversion.

6-4 Comparaison with Norcross and Seaton's method

Norcross and Seaton's method (1970) contains the hypothesis (see formula (4.3))

$$U_{ik}(r) = 0 \qquad \text{for} \quad r \geq r_0 \tag{6.6}$$

Hence there is no need of a first diagonalisation ($\mathcal{O} \equiv 1$)
The diagonal elements λ_i are

$$\lambda_i = l_i \tag{6.7}$$

By following the same method as in chapter IV they obtain the $\underset{\sim}{\chi}$ matrix and the χ'_{cc} matrix . The complex quantum defect is defined similarly .

Under the threshold it is possible to fit the $\mathcal{S}_{11}$ element to the profile formula (see (4.43))

$$\mathcal{S}_{11} = \alpha + \sum_r \frac{\beta_r}{e^{-2\pi i\nu} - \chi'_{rr}} \tag{6.8}$$

from which is deduced μ_r : $\chi'_{rr} = e^{2\pi i\mu_r}$.

Norcross and Seaton used a different fitting :

$$\begin{aligned} \mathcal{S}_{11} &= e^{2i\delta_1} \\ \delta_1 &= a + \sum_r \tan^{-1}\left(\frac{\frac{1}{2}\Gamma_r}{E_r - E}\right) \end{aligned} \tag{6.9}$$

The profile parameters were estimated by considering few energies over the resonances where the coupled equations were solved .

From E_r they deduced d_r :

$$E_r = E^{+}_{2p} - \frac{1}{2(n-d_r)^2} \tag{6.10}$$

and the complex quantum defect $\mu_r = \alpha_r + i\,\beta_r$:

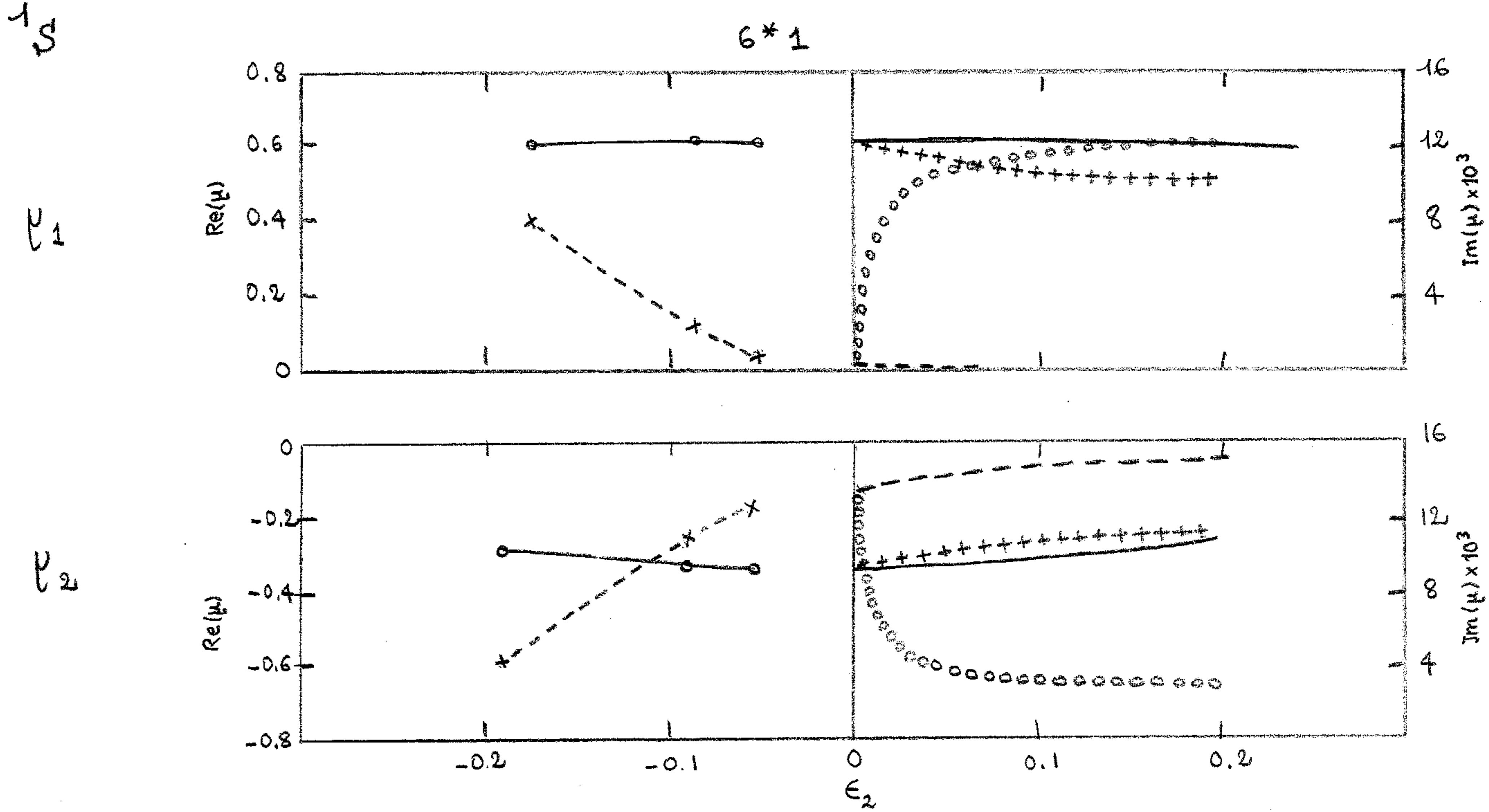
$$\left.\begin{aligned} (n-d_r)^2 &= \left[(n-\alpha_r)^2+\beta_r^2\right]^2 \Big/ \left[(n-\alpha_r)^2-\beta_r^2\right]^2 \\ \Gamma_r &= 2\,(n-\alpha_r)\,\beta_r \Big/ \left[(n-\alpha_r)^2+\beta_r^2\right]^2 \end{aligned}\right\} \tag{6.11}$$

We compared the two former methods . The results obtained were practically identical .

On figures 6*1 to 6*5 we plot the results obtained . Under the threshold the fitting method was used . Above the threshold (++++ , oooo) were obtained using Norcross and Seaton's method and (——— , - - - -) using chapter IV theory .

The comparaison of the results shows that an extrapolation from Norcross and Seaton's results is not good but from chapter IV theory it is very satisfactory except for the imginary part of the complex quantum defect for the last ~~table~~ figure . This imaginary part being very small it is possible that some numerical inaccuracies have produced the strange curve .

****

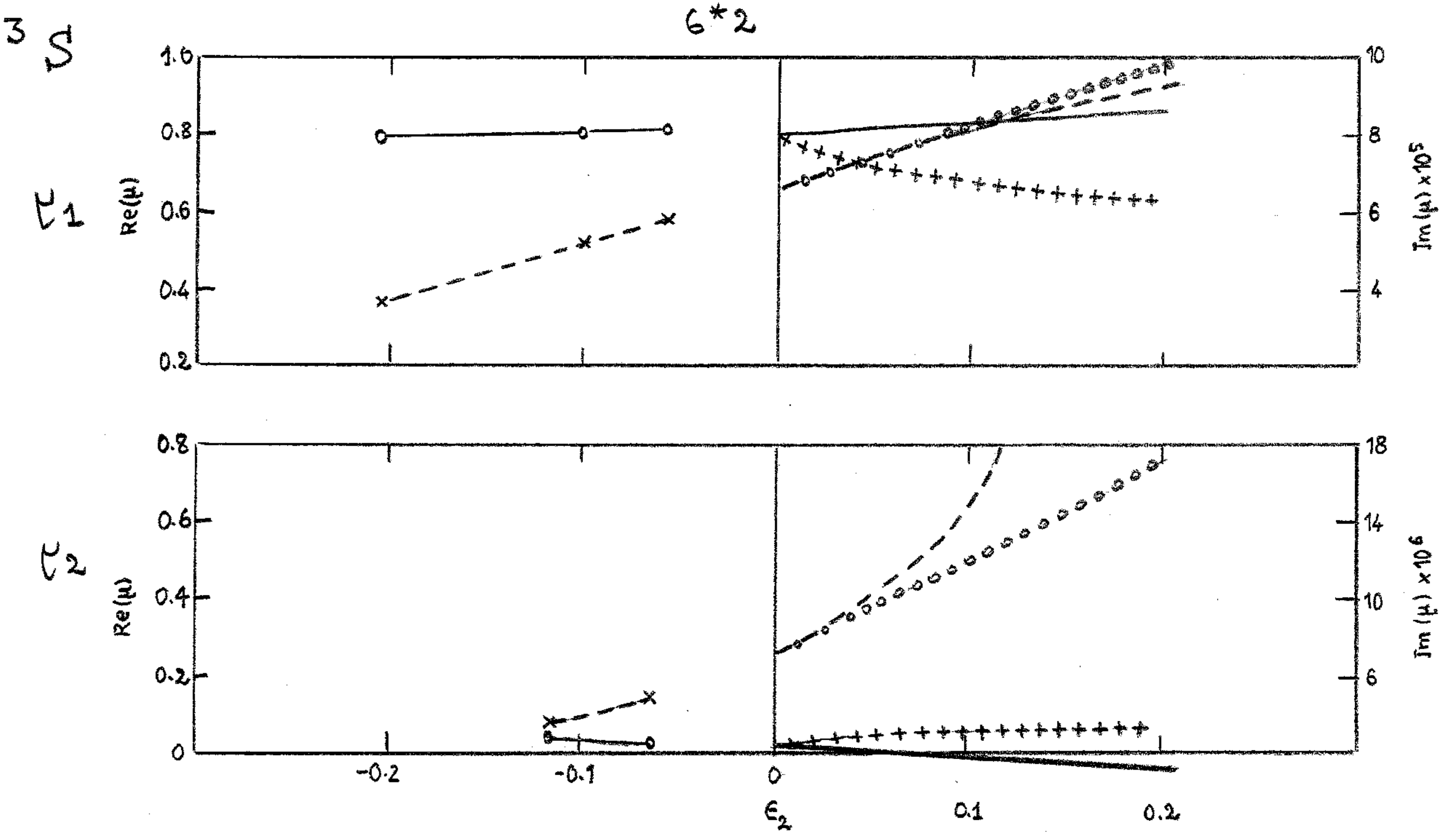


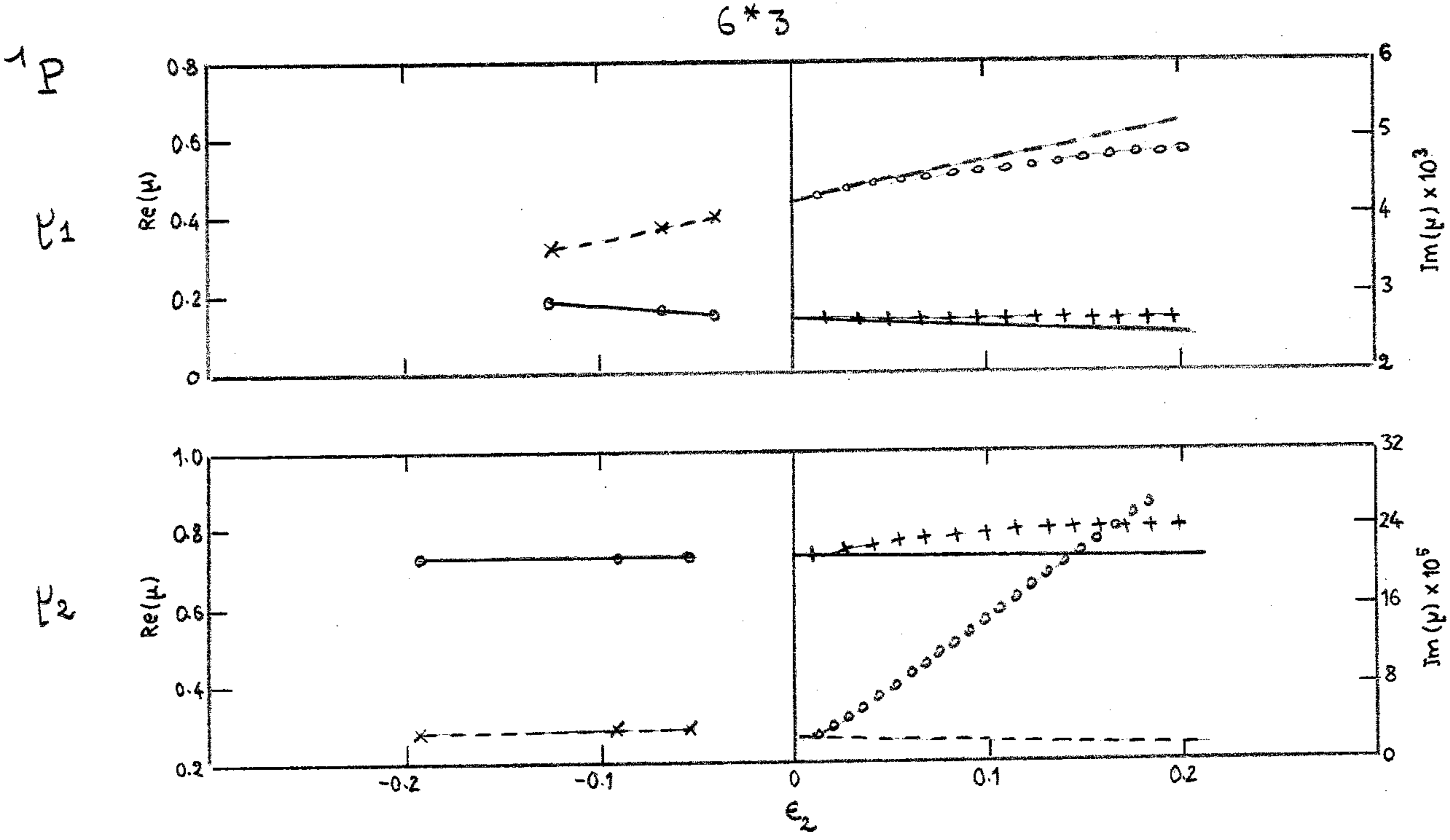
Complex quantum defects for He^+ scattering:

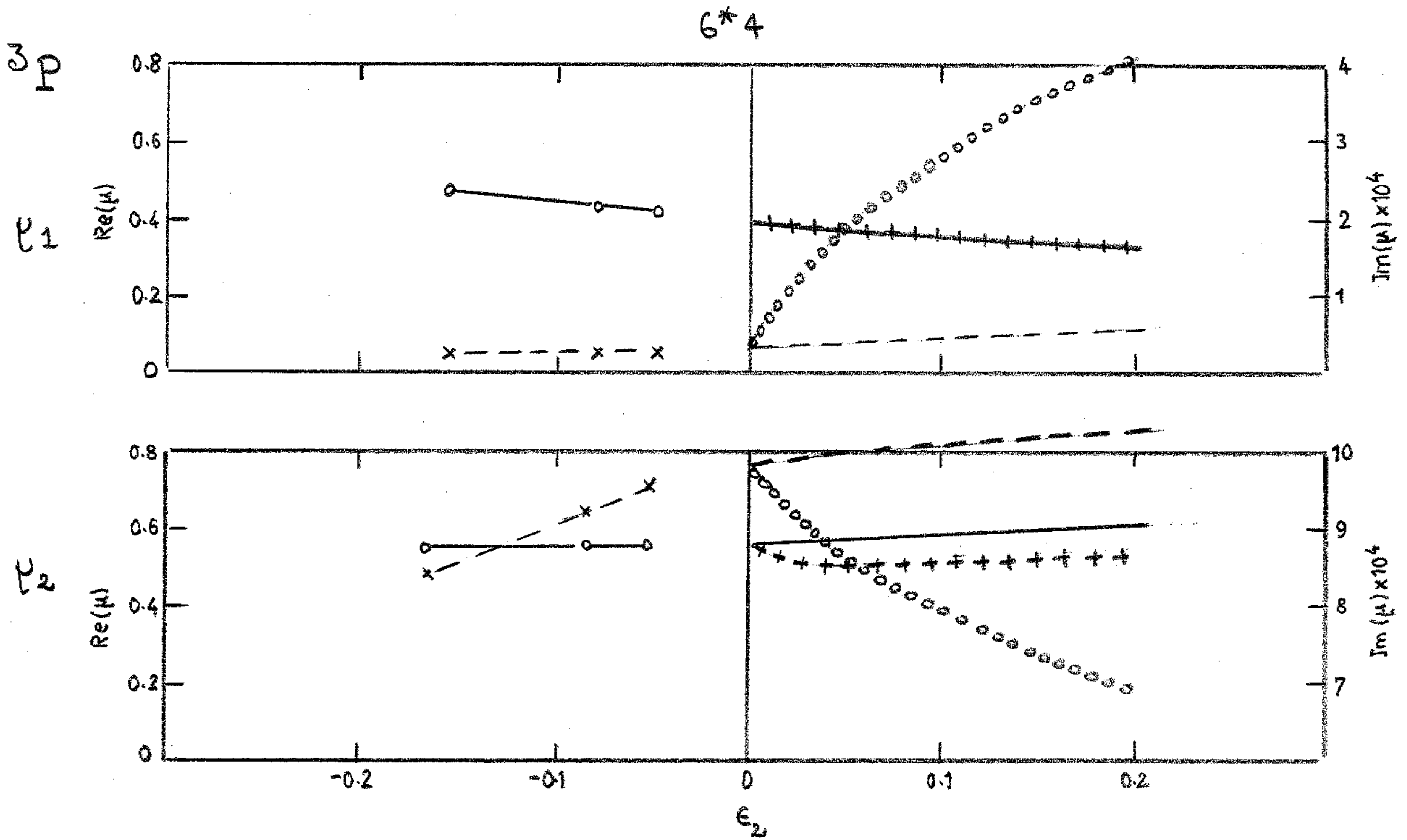
Real part of μ, left hand scale, +++++ Norcross, ——— present work

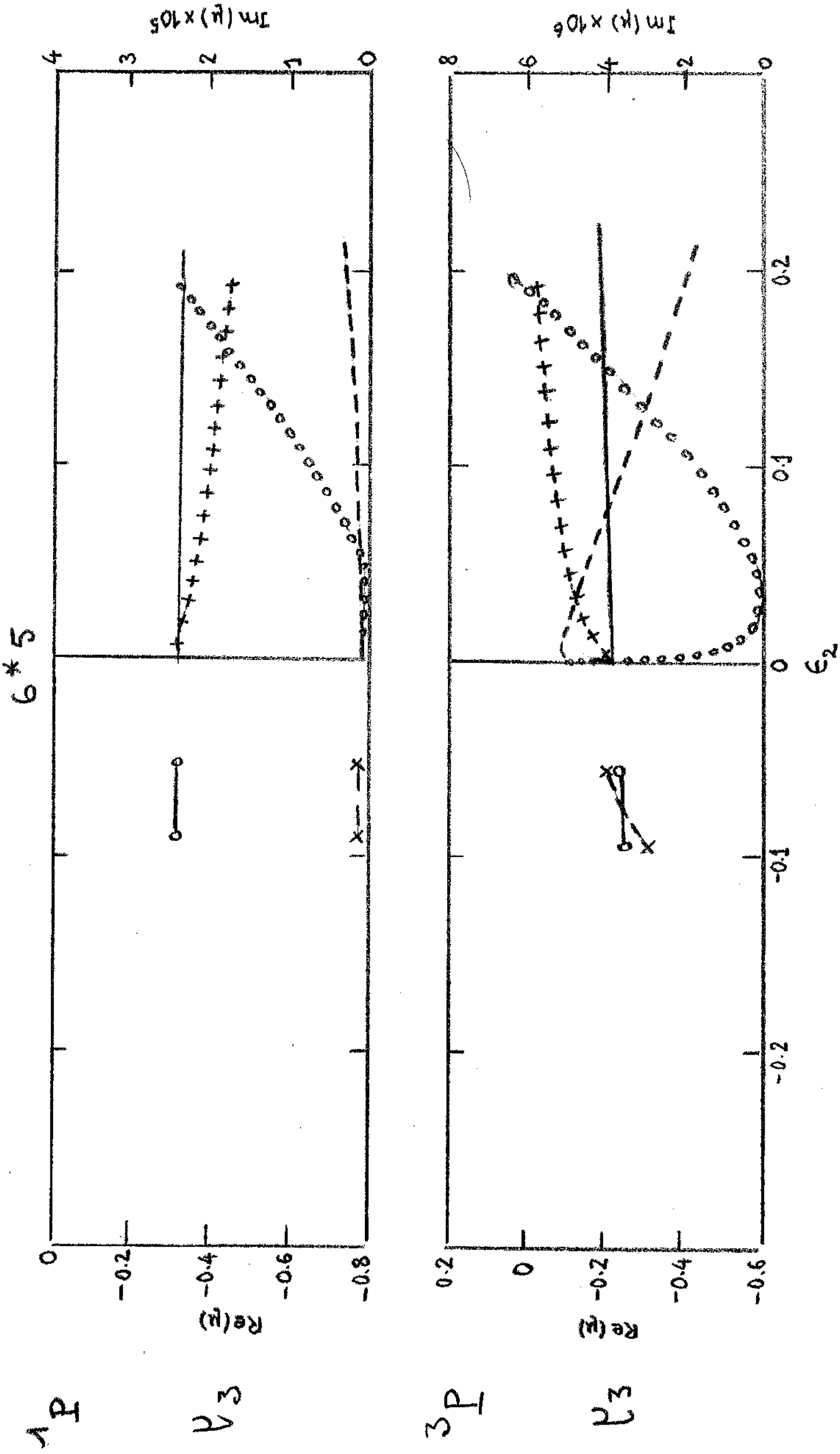
imaginary part of μ, right hand scale, ooooo Norcross, - - - - - present work.

From the profile fitting : real μ, o ; imaginary μ, x


3 S
6*2
τ1
Re(μ)
1.0
0.8
0.6
0.4
0.2
Im(μ) × 10^5
10
8
6
4
τ2
Re(μ)
0.8
0.6
0.4
0.2
0
Im(μ) × 10^6
18
14
10
6
-0.2
-0.1
0
ε2
0.1
0.2


6*3
^1P
μ_1
μ_2
Re(μ)
0
0.2
0.4
0.6
0.8
1.0
Im(μ) × 10³
2
3
4
5
6
Im(μ) × 10⁵
0
8
16
24
32
-0.2
-0.1
0
0.1
0.2
ε₂


6*4
3P
τ1
τ2
Re(μ)
Im(μ)×10⁴
0.8
0.6
0.4
0.2
0
4
3
2
1
10
9
8
7
-0.2
-0.1
0
0.1
0.2
ε2


6*5
¹P
ν₃
³P
ν₃
Re (μ)
Im (μ) × 10⁵
Im (μ) × 10⁶
ε₂
0
-0.2
-0.4
-0.6
-0.8
0.2
4
3
2
1
8
6
-0.2
-0.1
0
0.1
0.2

6*6

^1S

		$\underset{\sim}{\mu}_1$		$\underset{\sim}{\mu}_2$		$\underset{\sim}{\Omega}$			
	Energies	real	imag.	real	imag	Ω_{11}	Ω_{12}	Ω_{21}	Ω_{22}
S	3.00	−0.399	0.322 −3	−0.331	0.137 −1	0.0867	0.915	0.915	0.0867
N	3.01	−0.404	0.600 −4	−0.325	0.140 −1	0.139	0.862	0.862	0.139
N	3.03	−0.408	0.212 −4	−0.320	0.142 −1	0.161	0.839	0.839	0.161
N	3.05	−0.412	0.533 −5	−0.315	0.143 −1	0.178	0.822	0.822	0.178
S	3.10	−0.422	0.154 −5	−0.301	0.147 −1	0.209	0.791	0.791	0.209
S	3.24	−0.436	0.281 −4	−0.256	0.152 −1	0.246	0.755	0.755	0.246
B	3.24	−0.437	0.278 −4	−0.256	0.152 −1	0.246	0.754	0.754	0.246

Complex quantum defects and $\underset{\sim}{\Omega}$ matrix obtained using $\underset{\sim}{R}$ matrices from Burke et al. (1964), $\underline{B}$, and D. Norcross (1970), $\underline{N}$.

The $\underline{S}$ results were obtained using Seaton's programme (1970)

6*7

^3S		ν_1		ν_2		$\underset{\sim}{\Omega}$			
	Energies	real	imag.	real	imag.	Ω_{11}	Ω_{12}	Ω_{21}	Ω_{22}
S	3.00	0.0259	0.750 -5	-0.195	0.667 -4	0.478	0.522	0.522	0.478
N	3.01	0.0169	0.734 -5	-0.188	0.682 -4	0.482	0.518	0.518	0.482
N	3.03	0.0103	0.836 -5	-0.185	0.713 -4	0.495	0.505	0.505	0.495
N	3.05	0.0040	0.957-5	-0.182	0.743 -4	0.510	0.490	0.490	0.510
S	3.10	-0.0108	0.143-4	-0.175	0.809-4	0.553	0.447	0.447	0.553
S	3.24	-0.0394	0.407-4	-0.152	0.867-4	0.737	0.263	0.263	0.737
B	3.24	-0.0397	0.396-4	-0.152	0.863-4	0.736	0.264	0.264	0.736

^1P

6*8

		ν_1		ν_2		ν_3	
	Energies	real	imag.	real	imag.	real	imag.
S	3.00	0.136	0.421 -2	-0.324	0.842 -6	-0.276	0.311 -4
N	3.01	0.133	0.424 -2	-0.328	0.113 -5	-0.272	0.329 -4
N	3.03	0.128	0.434 -2	-0.328	0.127 -5	-0.271	0.320 -4
N	3.05	0.124	0.445 -2	-0.329	0.146 -5	-0.270	0.308 -4
S	3.10	0.116	0.472 -2	-0.332	0.195 -5	-0.267	0.275 -4
S	3.24	0.102	0.531 -2	-0.335	0.260 -5	-0.257	0.141 -4
B	3.24	0.101	0.531 -2	-0.335	0.243 -5	-0.257	0.137 -4

^1P

		6*9 $\underset{\sim}{\Omega}$								
	Energies	Ω_{11}	Ω_{12}	Ω_{13}	Ω_{21}	Ω_{22}	Ω_{23}	Ω_{31}	Ω_{32}	Ω_{33}
S	3.00	0.205	0.101	0.694	0.202	0.789	0.00906	0.593	0.1100	0.297
N	3.01	0.203	0.138	0.659	0.203	0.774	0.0234	0.594	0.0878	0.318
N	3.03	0.199	0.132	0.670	0.202	0.777	0.0213	0.600	0.0916	0.309
N	3.05	0.194	0.124	0.682	0.201	0.780	0.0189	0.605	0.0961	0.300
S	3.10	0.183	0.105	0.712	0.200	0.787	0.0131	0.617	0.1082	0.275
S	3.24	0.153	0.064	0.783	0.200	0.800	0.0036	0.650	0.136	0.214
B	3.24	0.153	0.064	0.783	0.197	0.800	0.0035	0.650	0.136	0.214

$6 * 10$

^3P

		ϱ_1		ϱ_2		ϱ_3	
	Energies	real	imag.	real	imag.	real	imag.
S	3.00	0.398	0.373 -4	-0.210	0.390 -5	-0.437	0.984 -3
N	3.01	0.395	0.344 -4	-0.212	0.492 -5	-0.428	0.992 -3
N	3.03	0.388	0.372 -4	-0.205	0.480 -5	-0.425	0.100 -2
N	3.05	0.381	0.404 -4	-0.200	0.455 -5	-0.421	0.101 -2
S	3.10	0.366	0.492 -4	-0.188	0.365 -5	-0.413	0.102 -2
S	3.24	0.333	0.787 -4	-0.166	0.138 -5	-0.390	0.104 -2
B	3.24	0.332	0.772 -4	-0.166	0.101 -5	-0.390	0.104 -2

^3P

6*11

		$\underset{\sim}{\Omega}$								
	Energies	Ω_{11}	Ω_{12}	Ω_{13}	Ω_{21}	Ω_{22}	Ω_{23}	Ω_{31}	Ω_{32}	Ω_{33}
S	3.00	0.144	0.347	0.508	0.388	0.537	0.075	0.467	0.116	0.417
N	3.01	0.138	0.345	0.517	0.385	0.537	0.078	0.477	0.118	0.405
N	3.03	0.133	0.351	0.516	0.388	0.531	0.081	0.479	0.118	0.403
N	3.05	0.130	0.357	0.513	0.391	0.525	0.084	0.480	0.118	0.402
S	3.10	0.122	0.370	0.508	0.396	0.512	0.092	0.482	0.118	0.400
S	3.24	0.105	0.400	0.495	0.408	0.482	0.110	0.487	0.117	0.396
B	3.24	0.105	0.401	0.494	0.409	0.482	0.110	0.486	0.117	0.396

6*12

^1D		ℓ_1		ℓ_2		ℓ_3	
	Energies	real	imag.	real	imag.	real	imag.
S	3.00	-0.0116	0.255 -3	-0.148	0.214 -6	0.253	0.758 -2
N	3.01	-0.0140	0.289 -3	-0.150	0.197 -6	0.258	0.766 -2
N	3.05	-0.0142	0.344 -3	-0.153	0.144 -7	0.257	0.803 -2
S	3.10	-0.0137	0.418 -3	-0.156	0.157 -6	0.256	0.846 -2
N	3.10	-0.0137	0.417 -3	-0.156	0.187 -6	0.256	0.845 -2
N	3.15	-0.0127	0.495 -3	-0.158	0.921 -6	0.257	0.884 -2
S	3.24	-0.0100	0.642 -3	-0.161	0.336 -5	0.260	0.942 -2
B	3.24	-0.0098	0.642 -3	-0.161	0.342 -5	0.260	0.939 -2

6*13

^1D

		$\underset{\sim}{\Omega}$								
	Energies	Ω_{11}	Ω_{12}	Ω_{13}	Ω_{21}	Ω_{22}	Ω_{23}	Ω_{31}	Ω_{32}	Ω_{33}
S	3.00	0.554	0.073	0.374	0.032	0.926	0.042	0.414	0.002	0.584
N	3.01	0.536	0.082	0.381	0.039	0.916	0.045	0.425	0.001	0.574
N	3.05	0.523	0.082	0.396	0.033	0.916	0.052	0.445	0.003	0.553
S	3.10	0.504	0.084	0.412	0.029	0.912	0.059	0.467	0.004	0.529
N	3.10	0.504	0.084	0.412	0.029	0.912	0.059	0.467	0.004	0.529
N	3.15	0.486	0.087	0.427	0.027	0.908	0.065	0.487	0.005	0.508
S	3.24	0.453	0.098	0.449	0.027	0.897	0.076	0.520	0.006	0.475
B	3.24	0.453	0.098	0.449	0.027	0.897	0.076	0.520	0.006	0.474

6*14

	^3D	ζ_1		ζ_2		ζ_3	
	Energies	real	imag.	real	imag.	real	imag.
S	3.00	0.105	0.178 -3	-0.136	0.350 -6	-0.491	0.156 -6
N	3.01	0.105	0.183 -3	-0.140	0.151 -6	-0.489	0.257 -6
N	3.05	0.107	0.667 -2	-0.138	0.742 -4	-0.496	0.186 -6
S	3.10	0.109	0.221 -3	-0.136	0.409 -7	-0.503	0.101 -6
N	3.10	0.109	0.221 -3	-0.136	0.403 -7	-0.504	0.121 -6
N	3.15	0.110	0.243 -3	-0.134	0.528 -8	-0.511	0.823 -7
S	3.24	0.110	0.271 -3	-0.130	0.115 -6	-0.523	0.689 -9
B	3.24	0.110	0.272 -3	-0.130	0.101 -6	-0.524	0.276 -8

6*15

^3D

		$\underset{\sim}{\Omega}$								
	Energies	Ω_{11}	Ω_{12}	Ω_{13}	Ω_{21}	Ω_{22}	Ω_{23}	Ω_{31}	Ω_{32}	Ω_{33}
S	3.00	0.494	0.171	0.336	0.133	0.825	0.042	0.373	0.004	0.622
N	3.01	0.479	0.181	0.340	0.142	0.814	0.044	0.379	0.006	0.616
N	3.05	0.454	0.199	0.347	0.153	0.795	0.052	0.393	0.006	0.601
S	3.10	0.426	0.220	0.355	0.167	0.773	0.060	0.408	0.007	0.586
N	3.10	0.425	0.220	0.355	0.167	0.773	0.060	0.408	0.007	0.586
N	3.15	0.400	0.238	0.362	0.179	0.754	0.067	0.420	0.008	0.571
S	3.24	0.363	0.256	0.372	0.200	0.723	0.076	0.437	0.011	0.551
B	3.24	0.362	0.256	0.372	0.200	0.723	0.077	0.438	0.011	0.551

6 * 16

^1F

		ζ_1		ζ_2		ζ_3	
	Energies	real	imag.	real	imag.	real	imag.
N	3.002	0.00030	0.173 -5	-0.0817	0.236 -7	0.0414	0.285 -3
S	3.005	0.00039	0.190 -5	-0.0812	0.317 -7	0.0413	0.290 -3
S	3.01	0.00035	0.210 -5	-0.0811	0.388 -7	0.0412	0.296 -3
N	3.01	0.00045	0.212 -5	-0.0810	0.420 -7	0.0413	0.296 -3
S	3.02	0.00001	0.264 -5	-0.0813	0.731 -7	0.0409	0.310 -3
N	3.10	-0.00282	0.862 -5	-0.0839	0.110 -5	0.0392	0.426 -3
B	3.24	-0.00553	0.171 -4	-0.0883	0.596 -5	0.0396	0.649 -3

^1F

6*17

		$\underset{\sim}{\Omega}$								
	Energie	Ω_{11}	Ω_{12}	Ω_{13}	Ω_{21}	Ω_{22}	Ω_{23}	Ω_{31}	Ω_{32}	Ω_{33}
N	3.002	0.909	0.052	0.039	0.053	0.947	0.0003	0.039	0.0009	0.961
S	3.005	0.910	0.052	0.039	0.052	0.947	0.0003	0.038	0.0009	0.962
S	3.01	0.912	0.051	0.037	0.052	0.948	0.0002	0.036	0.0009	0.963
N	3.01	0.912	0.051	0.037	0.051	0.948	0.0002	0.036	0.0009	0.963
S	3.02	0.916	0.049	0.034	0.050	0.950	0.0001	0.034	0.0010	0.965
N	3.10	0.941	0.037	0.023	0.039	0.961	0.0005	0.021	0.0026	0.977
B	3.24	0.954	0.023	0.023	0.026	0.971	0.0028	0.020	0.0057	0.975

6 * 18

^3F		ζ_1		ζ_2		ζ_3	
	Energies	real	imag.	real	imag.	real	imag.
N	3.002	0.00802	0.712 -5	-0.0813	0.447 -8	0.232	0.504 -3
S	3.005	0.00831	0.737 -5	-0.0808	0.532 -8	0.232	0.506 -3
N	3.01	0.00877	0.791 -5	-0.0806	0.381 -8	0.233	0.508 -3
S	3.01	0.00867	0.791 -5	-0.0806	0.473 -8	0.233	0.509 -3
S	3.02	0.00905	0.889 -5	-0.0807	0.282 -8	0.234	0.514 -3
N	3.10	0.0120	0.184 -4	-0.0817	0.747 -8	0.242	0.544 -3
B	3.24	0.0167	0.416 -4	-0.0821	0.437 -7	0.246	0.565 -3

^3F

		6*19								
		$\underset{\sim}{\Omega}$								
	Energies	Ω_{11}	Ω_{12}	Ω_{13}	Ω_{21}	Ω_{22}	Ω_{23}	Ω_{31}	Ω_{32}	Ω_{33}
N	3.002	0.727	0.065	0.208	0.053	0.934	0.012	0.220	0.00011	0.780
S	3.005	0.725	0.066	0.209	0.053	0.934	0.013	0.222	0.00009	0.778
N	3.01	0.722	0.066	0.212	0.053	0.934	0.013	0.225	0.00007	0.775
S	3.01	0.722	0.066	0.212	0.053	0.934	0.013	0.225	0.00007	0.775
S	3.02	0.716	0.067	0.217	0.053	0.933	0.014	0.232	0.00004	0.768
N	3.10	0.669	0.077	0.254	0.057	0.923	0.020	0.274	0.00001	0.726
B	3.24	0.602	0.099	0.299	0.069	0.901	0.030	0.329	0.00009	0.671

6*20

	^1G	ν_1		ν_2		ν_3	
	Energies	real	imag.	real	imag.	real	imag.
S	3.005	0.00127	0.261 -7	-0.0507	0.275 -8	0.0535	0.108 -4
S	3.01	0.00132	0.296 -7	-0.0507	0.132 -9	0.0536	0.115 -4
N	3.01	0.00136	0.219 -7	-0.0536	0.125 -9	0.0537	0.114 -4
S	3.02	0.00142	0.223 -7	-0.0509	0.309 -11	0.0534	0.128 -4
N	3.10	0.00129	0.606 -7	-0.0522	0.193 -7	0.0508	0.257 -4
B	3.24	0.00090	0.107 -6	-0.0543	0.176 -6	0.0407	0.569 -4
DW	3.01	0.00339	0.660 -7	-0.00500	0.479 -9	-0.0153	0.134 -4

D.W. : Distorted wave Approximation of Eissner et al. (1969)

^1G

6*21

		$\underset{\sim}{\Omega}$								
	Energies	Ω_{11}	Ω_{12}	Ω_{13}	Ω_{21}	Ω_{22}	Ω_{23}	Ω_{31}	Ω_{32}	Ω_{33}
S	3.005	0.887	0.037	0.076	0.036	0.963	0.0016	0.077	0.00021	0.923
S	3.01	0.887	0.037	0.076	0.036	0.963	0.0016	0.077	0.00022	0.923
N	3.01	0.875	0.037	0.088	0.036	0.962	0.0021	0.090	0.00017	0.910
S	3.02	0.887	0.036	0.077	0.035	0.964	0.0014	0.078	0.00025	0.922
N	3.10	0.851	0.036	0.113	0.034	0.964	0.0019	0.115	0.00048	0.885
B	3.24	0.893	0.027	0.080	0.029	0.971	0.00003	0.078	0.00251	0.920
DW	3.01	0.986	0.006	0.008	0.006	0.994	0.00007	0.008	0.000003	0.992

6*22

^3G		ψ_1		ψ_2		ψ_3	
	Energies	real	imag.	real	imag.	real	imag.
S	3.005	0.00151	0.174 -7	-0.0507	0.361 -9	0.0621	0.134 -4
S	3.01	0.00158	0.216 -7	-0.0507	0.429 -9	0.0626	0.142 -4
N	3.01	0.00171	0.266 -7	-0.0506	0.173 -9	0.0627	0.142 -4
S	3.02	0.00176	0.334 -7	-0.0509	0.363 -10	0.0632	0.159 -4
N	3.10	0.00231	0.169 -6	-0.0520	0.168 -7	0.0672	0.313 -4
B	3.24	0.00365	0.104 -5	-0.0536	0.878 -7	0.0740	0.653 -4
DW	3.01	0.00364	0.983 -8	-0.00500	0.378 -8	-0.00379	0.810 -5

6*23

^3G

		$\underset{\sim}{\Omega}$								
	Energies	Ω_{11}	Ω_{12}	Ω_{13}	Ω_{21}	Ω_{22}	Ω_{23}	Ω_{31}	Ω_{32}	Ω_{33}
S	3.005	0.887	0.037	0.076	0.036	0.963	0.0016	0.077	0.00021	0.923
S	3.01	0.887	0.037	0.076	0.036	0.963	0.0016	0.077	0.00021	0.923
N	3.01	0.891	0.033	0.076	0.032	0.966	0.0015	0.077	0.00017	0.923
S	3.02	0.887	0.036	0.077	0.035	0.963	0.0014	0.078	0.00025	0.922
N	3.10	0.888	0.032	0.081	0.032	0.967	0.0005	0.080	0.00092	0.919
B	3.24	0.809	0.038	0.152	0.037	0.961	0.0026	0.154	0.00084	0.845
D W	3.01	0.993	0.007	0.001	0.006	0.993	0.0008	0.0009	0.0007	0.998

6 * 24

			ξ_1		ξ_2		ξ_3	
		Energies	real	imag.	real	imag.	real	imag.
^1H	D W	3.01	0.00247	0.174 -8	-0.00343	0.405 -8	-0.00240	0.244 -6
^3H	D W	3.01	0.00249	0.203 -8	-0.00343	0.174 -8	-0.00207	0.203 -6

			$\underset{\sim}{\Omega}$								
		Energies	Ω_{11}	Ω_{12}	Ω_{13}	Ω_{21}	Ω_{22}	Ω_{23}	Ω_{31}	Ω_{32}	Ω_{33}
^1H	D W	3.01	0.993	0.00431	0.00282	0.00327	0.975	0.0217	0.00386	0.0206	0.976
^3H	D W	3.01	0.991	0.00430	0.00501	0.00327	0.984	0.0130	0.00604	0.0120	0.982

6 * 25

			ν_1		ν_2		ν_3	
		Energies	real	imag.	real	imag.	real	imag.
^1I	D W	3.01	0.0016	0.337 -10	-0.002	0.522 -10	-0.0005	0.307 -8
^3I	D W	3.01	0.0016	0.339 -10	-0.002	0.517 -10	-0.0005	0.307 -8

			$\underset{\sim}{\Omega}$								
		Energies	Ω_{11}	Ω_{12}	Ω_{13}	Ω_{21}	Ω_{22}	Ω_{23}	Ω_{13}	Ω_{23}	Ω_{33}
^1I	D W	3.01	0.976	0.0154	0.0090	0.0182	0.968	0.0139	0.00616	0.0167	0.977
^3I	D W	3.01	0.976	0.0154	0.0090	0.0182	0.968	0.0137	0.00621	0.0165	0.977

CHAPTER VII

Calculation of the dielectronic recombination rate

For obtaining the dielectronic recombination we have to choose some energy probability distribution for the colliding electron . It is usually considered that it is a Maxwell distribution . Then we can deduce that for $He^+ + e^-$ the dielectronic recombination is important for a temperature around $T \sim 10^5 \,°K$.

The dielectronic recombination depends also of the electron density . When this density increases the ionization of the high excited states of He decreases the recombination probability Burgess and Summers evaluated that for $N_e \sim 10^8 cm^{-2}$ this ionization effect is still very small .

7-1 Formulation of the problem

Let's consider an electron having a velocity v and forming with $He^+(1s)$ a system having the quantum numbers L , S The capture cross section σ_v that the former system is captured into the "states" $1s(\nu\ell+1)_{2p}$ or $1s(\nu\ell-1)_{2p}$ is (using (5.30) or (5.49)) :

$$\sigma_{v} = \frac{\pi}{2\omega^{+}} \left(\frac{\hbar}{mv}\right)^{2} (2L+1)(2S+1) \left| S^{(p,e)}_{LS} \right|^{2} \tag{7.1}$$

$2\omega^{+}$ is the statistical weight of the initial state : $He^{+}(1s) + e^{-}$. ($2\omega^{+} = 4$)

The Maxwell distribution density is

$$f(v) = 4\pi v^{2} \left(\frac{m}{2kT}\right)^{3/2} e^{-\frac{mv^{2}}{2kT}} \tag{7.2}$$

k is the Maxwell Boltzmann constant . T is the temperature $f(v)$ is a normalised density :

$$\int f(v)\, dv = 1 \tag{7.3}$$

The dielectronic recombination rate into $1s\, n\ell\pm1$, is by definition

$$\alpha_{d}(n\ell\pm1) = \sum_{p} \int \sigma_{v}^{(np)}\, v\, f(v)\, dv \tag{7.4}$$

The symbol n represents the summation on p consecutive resonances i.e. summation over the resonances having the same principal quantum number n .

This gives using the energy relation $E = \frac{mv^{2}}{2}$

$$\alpha_{d}(n\ell\pm1) = 2\left(\frac{2}{\pi m}\right)^{1/2} \left(\frac{1}{kT}\right)^{3/2} \sum_{p} \int \sigma_{v}^{(np)} E\, e^{-\frac{E}{kT}}\, dE \tag{7.5}$$

The resonance np being very narrow we can consider that $e^{-\frac{E}{kT}}$ is practically constant over the resonance .

$$\left.\begin{aligned} E &\simeq E_{np} \\ E_{np} &= E^{+}_{2p} - \frac{1}{2\nu^2_{np}} \end{aligned}\right\} \qquad (7.6)$$

In the purpose to obtain a formula independant of the unit system we have to.transform (5.31) and (5.53) as follow :

$$\left.\begin{aligned} \underline{P}^1(np) &= \frac{2\pi\, B_p^{(LS)+} B_p^{(LS)} A_{np}^{(LS)}}{B_p^{(LS)+} B_p^{(LS)} + A_{np}^{(LS)}} \\ \underline{P}^2(np) &= \frac{2\pi\, B_p^{(LS)+} B_p^{(LS)} A_{np}^{(LS)}}{B_p^{(LS)+} B_p^{(LS)} + A_{np}^{(LS)} \left(1 - \frac{\pi}{2} \nu^3_{np} B_p^{(LS)+} B_p^{(LS)}\right)^2} \end{aligned}\right\} \qquad (7.7)$$

and define the autoionisation probability by

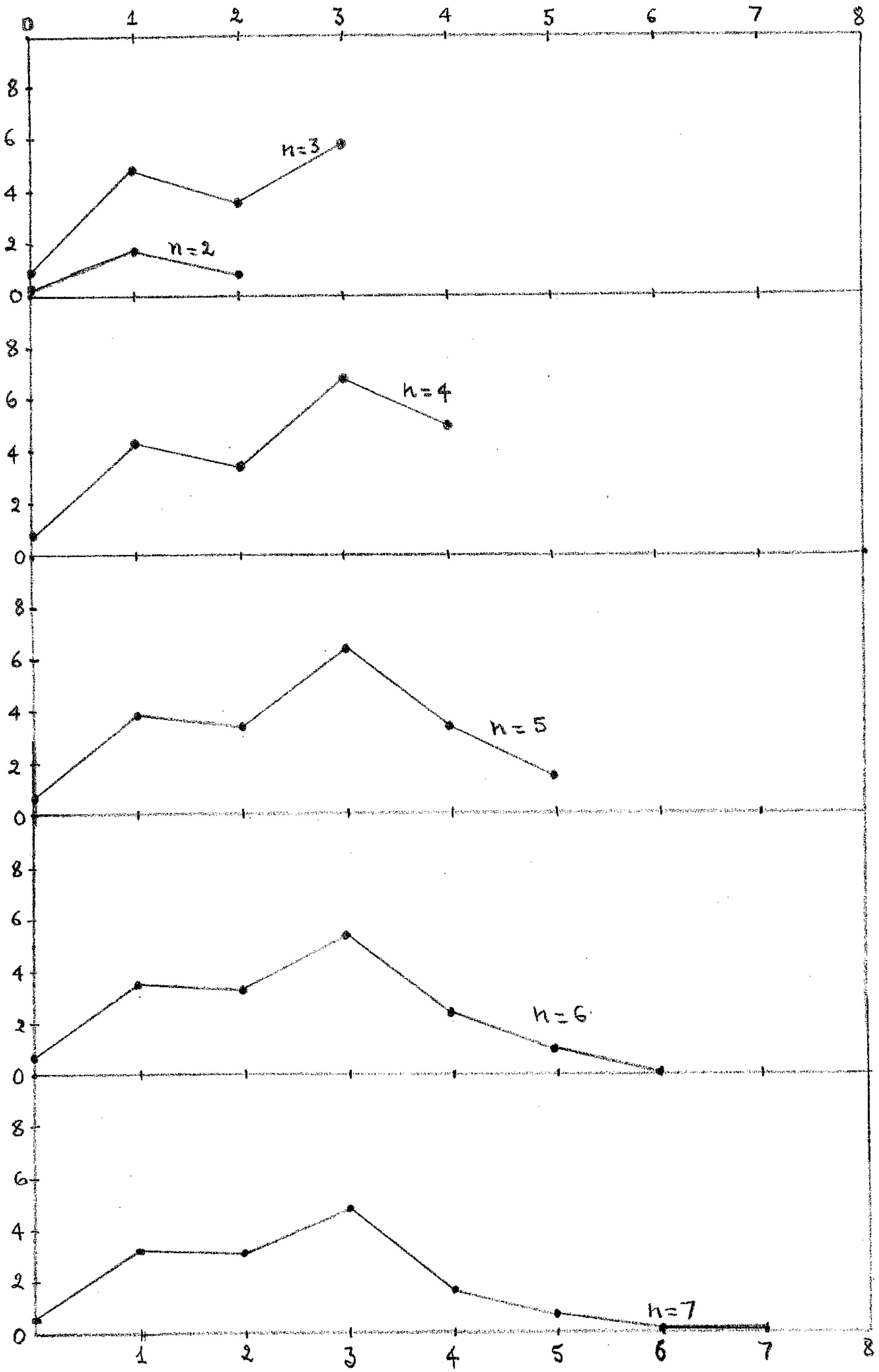
$$A_{np}^{(LS)} = \frac{\Gamma_{np}^{(LS)}}{\hbar} \qquad (7.8)$$

Hence

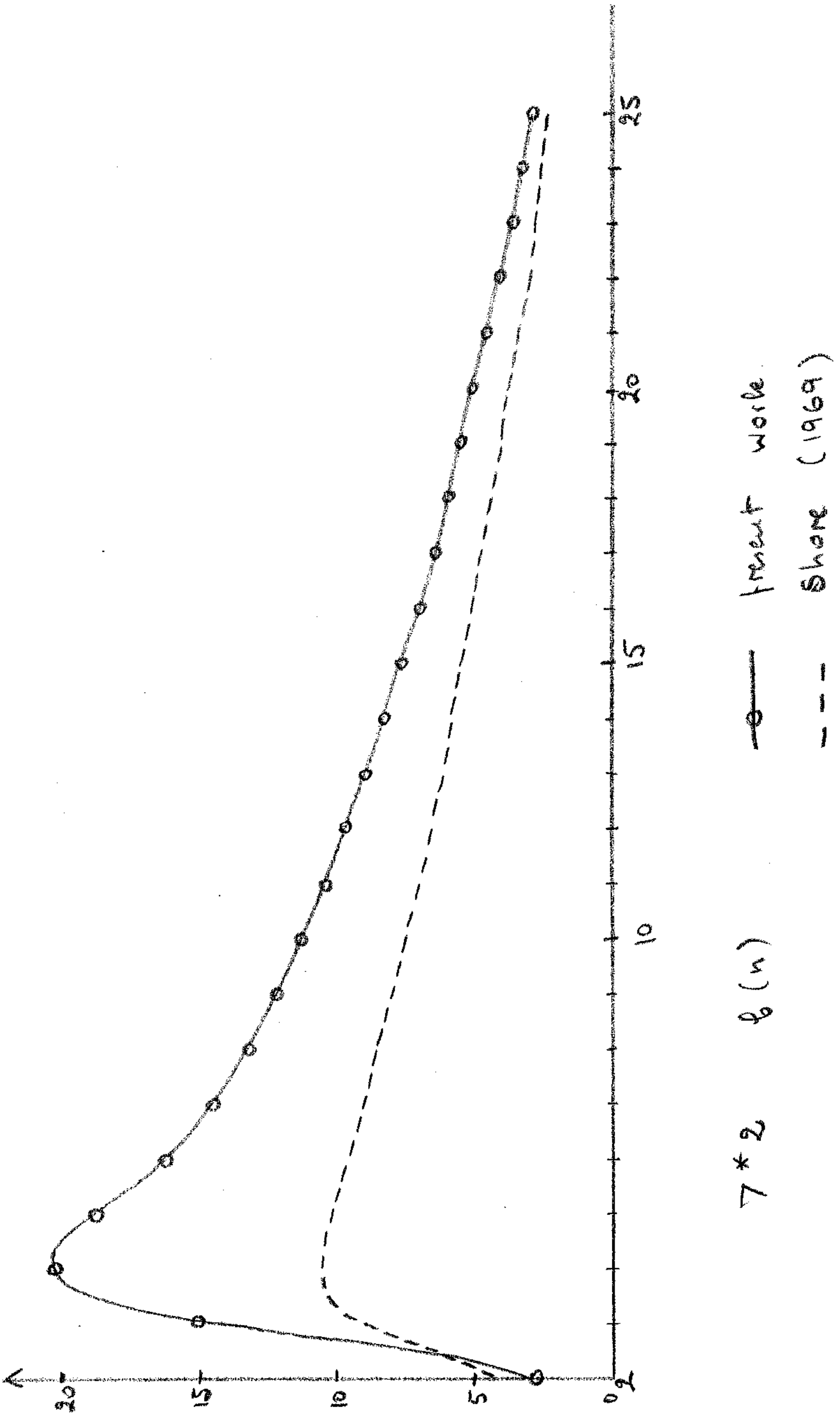
$$\alpha_d(n\ell \pm 1) = \frac{(2L+1)(2S+1)}{2\omega^{+}} \frac{h^3}{(2\pi m kT)^{3/2}} \sum_p e^{-\frac{E_{np}}{kT}}\ \underline{P}\,(np) \qquad (7.9)$$

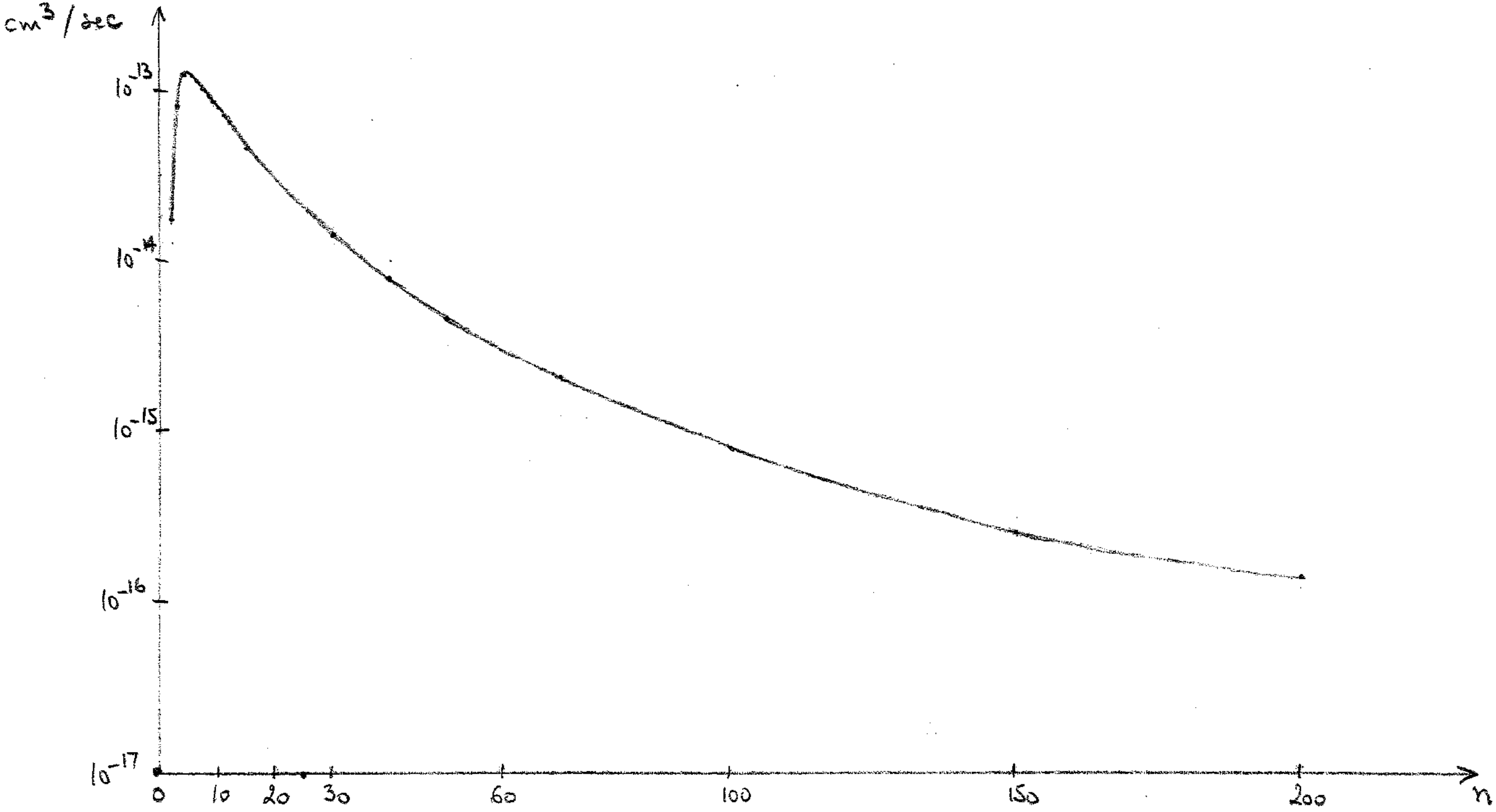
This formula is similar to the one obtained by Bates and Dalgarno in 1962 .

7-2 Results



7*1 b(nL) in function of L


7*2
b(n)
present work
Shore (1969)
0
5
10
15
20
0
10
15
20
25



7 * 3 $\alpha_d(n)$ for T = 250000 °K

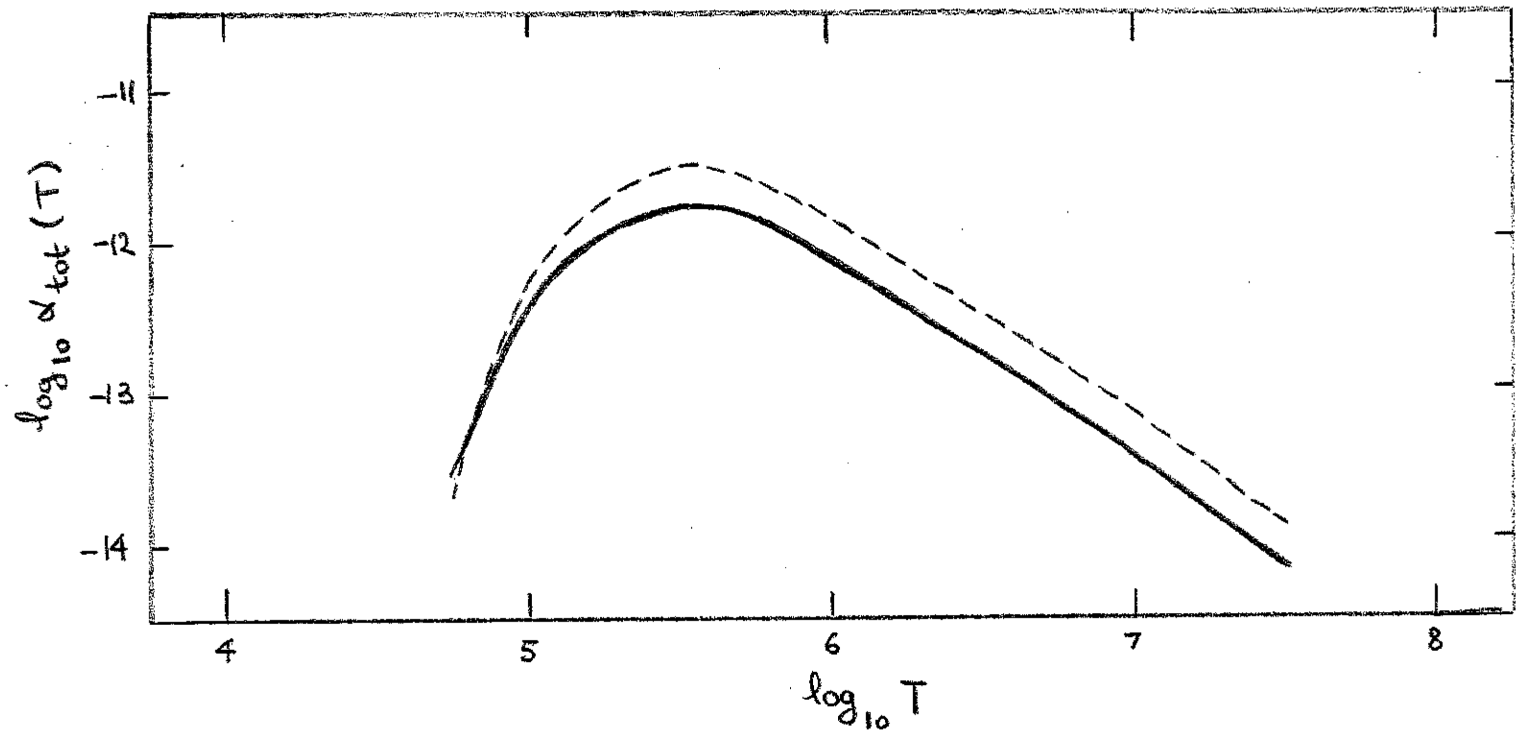
Temperature $T = 250000\,^\circ K$

	$\alpha_d^1(n)$	$\alpha_d^2(n)$
$n = 10$	5.566 -14	5.568 -14
$n = 20$	2.563 -14	2.569 -14
$n = 50$	4.703 -15	4.772 -15
$n = 100$	8.152 -16	8.353 -16
$n = 150$	2.617 -16	2.675 -16
$n = 200$	1.137 -16	1.148 -16
$n = 600$	4.317 -18	2.852 -18
$n = 1000$	9.329 -19	3.414 -19
$n = 3000$	3.455 -20	1.517 -21
$n = 5000$	7.462 -21	9.862 -23
Σ_n	1.482 -12	1.487 -12

7*4 Dielectronic recombination rates

$\alpha_d^1(n)$, $\alpha_d^2(n)$ corresponding to

$P^1(np)$, $P^2(np)$



7*5 He$^+$+e Dielectronic recombination coefficient

α_{tot} (T) (cm^3 sec^{-1})

——— : present work

- - - - : Burgers (1964)

In the purpose to be able to compare the following results to those of Shore (1969) and Burgess and Summers (1969) we shall define equivalent quantities that we shall plot .

Corresponding to the formula (38) of Shore we define :

$$b(nL) = \frac{(2L+1)}{2\omega^{+} A_r} \sum_{S} (2S+1) \sum_{p} \frac{B_p^{(LS)+} B_p^{(LS)} A_{np}^{(LS)}}{A_{np}^{(LS)} + B_p^{(LS)+} B_p^{(LS)}} \qquad (7.10)$$

A_r is related to $B_p^{+} B_p$ by :

$$\sum B_p^{(LS)+} B_p^{(LS)} \simeq f A_r \qquad (7.11)$$

where $f=1$ for $L=0$

$f=2$ for $L\neq 0$

The left and right hand side are nearly equal for $\underset{\sim}{X}$ is nearly unitary . (see (4.60))

Burgess and Summers and Shore plot $b(n)$:

$$b(n) = \sum_{L} b(nL) \qquad (7.12)$$

On figure 7*1 we give our results for $b(nL)$ for $n=2$ to 7. On figure 7*2 we plot $b(n)$ obtained by our method and by Shore . On figure 7*3 we give $\alpha_d(n)$

$$\alpha_d(n) = \sum_{LS} \alpha_d(n\ell \pm 1) \qquad (7.13)$$

We also computed $\alpha_d(n)$ using the "overlap correction" developped in 5-1 . The correction is very small and is not large enough to be significant.

We did some computations replacing $P^1(np)$ by $P^2(np)$ into (7.9) . The results become different only for n large , as expected . We give some results in table 7*4 corresponding to the temperature $T = 250000^\circ K$.

On figure 7*5 we compare the total recombination rate

$$\alpha_{tot}(T) = \sum_n \alpha_d(n,T) \qquad (7.14)$$

with Burgess' results (1964) . Burgess also included the recombination from $n = 3$, ... This contribution is of the order of 10 % of the recombination from $n = 2$ whereas the difference between our results and those of Burgess is significantly larger than this correction .

****

CHAPTER VIII

Conclusion

In the earlier chapters we gave a theory as well as a method for computing the dielectronic recombination quantities in the case where there is a strong coupling between the degenerate closed channels . In the case where we should have non degenerate target states the method could be simplified for we should not need any diagonalisation for the asymptotic potential .

The results obtained for He^+ are in between those of Burgess and Shore . We think that Burgess overevaluated the autoionisation probabilities using the Bethe Approximation and Shore under estimated by neglecting some "small integrals" and the interaction probabilities between closed channels (configuration interaction between resonances) .

****

Appendix 1

Study of $A(\epsilon,\lambda)$

$A(\epsilon,\lambda)$ is defined by (4.14) . For $\lambda = \ell$ it is possible to express $\Gamma(K+\ell+1)$ and $\Gamma(K-\ell)$ in function of $\Gamma(K)$ using the canonical relation

$$\Gamma(x+1) = x\,\Gamma(x) \qquad (A1)$$

and to obtain the polynom

$$A(\epsilon,\ell) = \prod_{p=0}^{\ell} (1+\epsilon p^2) \qquad (A2)$$

We are only interested by a very small energy region , just above and under the threshold . We can consider only the first order of the polynoms :

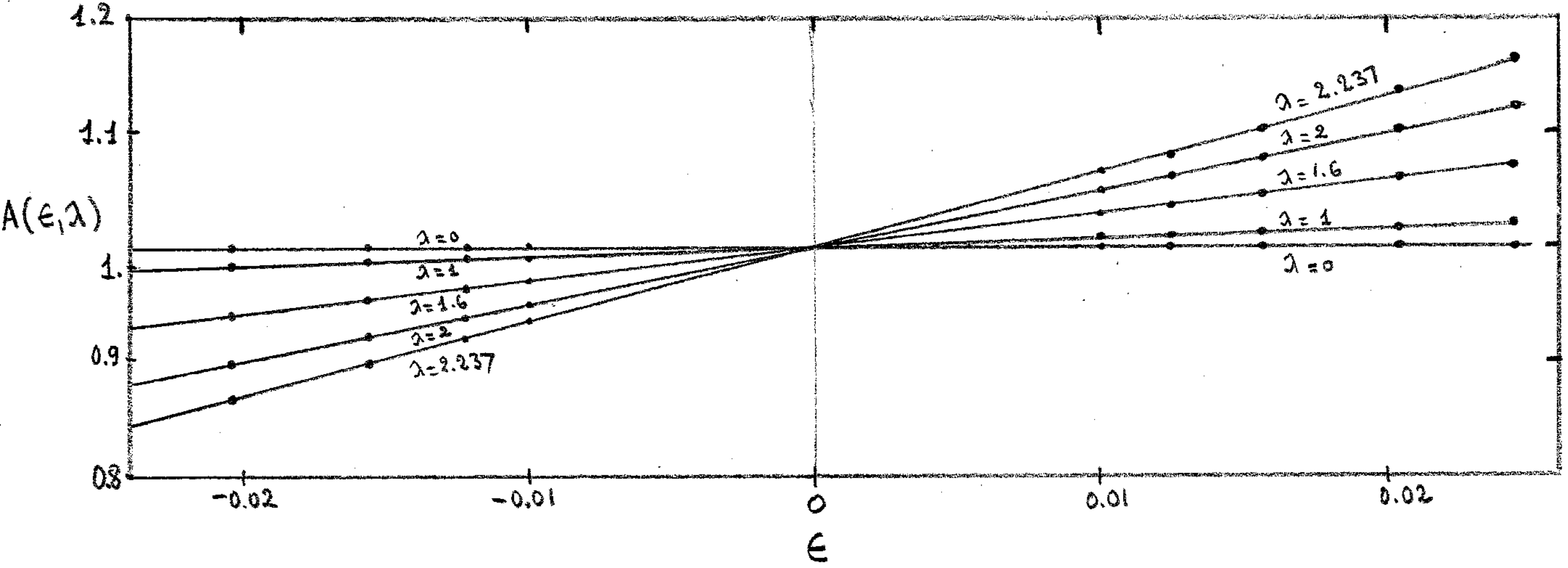
for $\ell = 0$ $A(\epsilon,0) = 1$

for $\ell = 1$ $A(\epsilon,1) = 1+\epsilon$

for $\ell = 2$ $A(\epsilon,2) \simeq 1+5\epsilon$

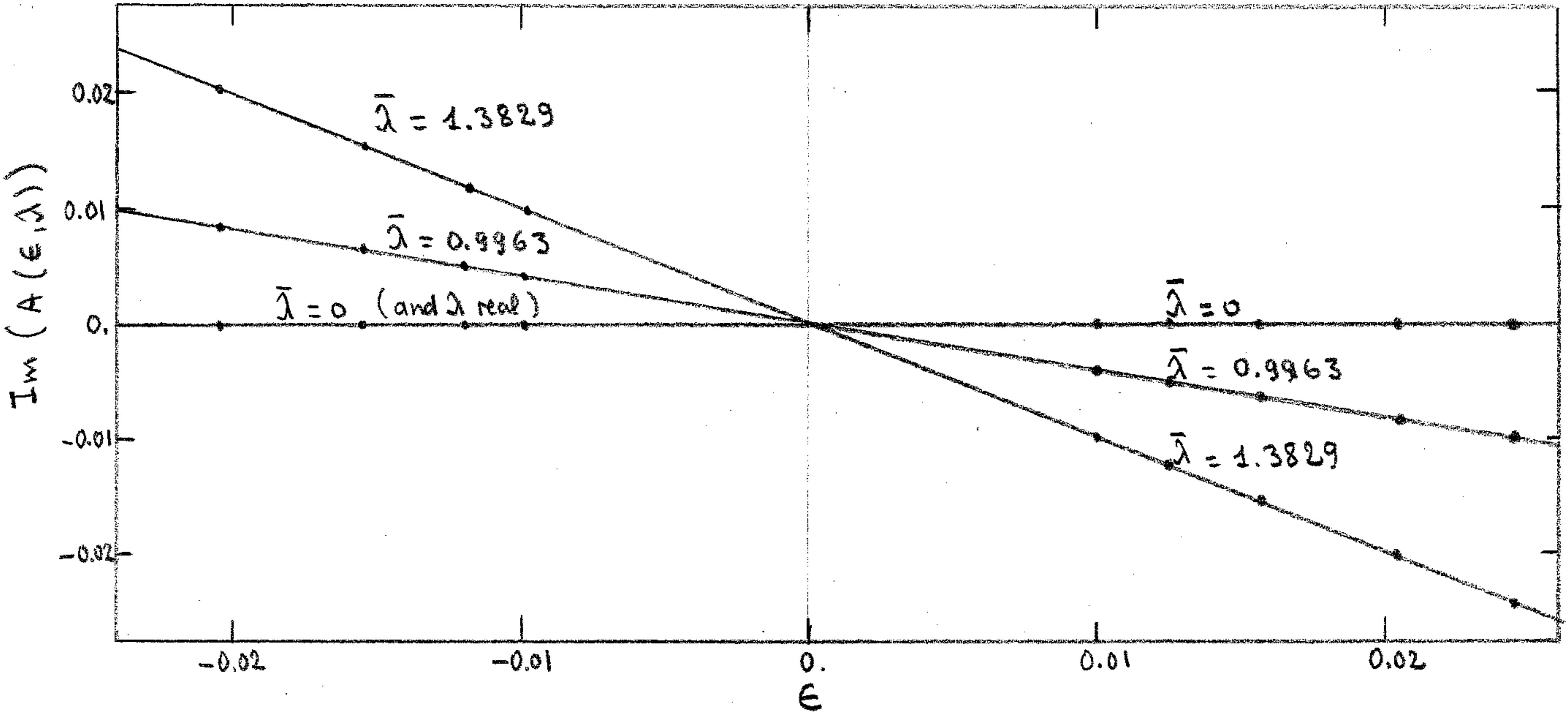
It is logical to think that for $\lambda = 1.6$, for exemple , $A(\epsilon,1.6) \simeq 1+\alpha\epsilon$ where $1 < \alpha < 5$.

We checked this idea by building a programme for computing $A(\epsilon,\lambda)$ for λ real and $\lambda = -\frac{1}{2}+i\tilde{\lambda}$. On figure A*1 we give the results obtained for $\lambda = 0, 1, 1.6, 2, 2.237$. We see that for



A*1 $A(\epsilon,\lambda)$ in function of ϵ and λ (real)

● : computed results



A^*2 : Imaginary part of $A(\epsilon, \lambda)$.
$\lambda = -\frac{1}{2} + i\bar{\lambda}$

ϵ between -0.02 and $+0.02$

$$A(\epsilon,\lambda) \simeq 1 + \alpha(\lambda)\,\epsilon \qquad (A3)$$

We also give the immaginary part of $A(\epsilon,\lambda)$ for $\lambda = -\frac{1}{2} + i\bar{\lambda}$ $\bar{\lambda} = 0,\ 0.9963,\ 1.3829$. The real part follows also the same pattern We deduce that (A3) is also valid for λ complex .

On a larger energy scale $A(\epsilon,\lambda)$ keeps good properties and we can deduce that $A(\epsilon,\lambda)$ is slowly varying .

****

Appendix 2

Study of $K(\nu,\lambda)$

$K(\nu,\lambda)$ is defined by (4.17) . We saw in formula (4.18) that $K(\nu,\lambda)$ was real and positive for any λ real or $\lambda = -\frac{1}{2} + i\tilde{\lambda}$. Now for $\lambda = \ell$ using the formula (A1) we have

$$K(\nu,\ell) = \frac{1}{\Gamma(\nu)\,\nu^{3/2}} \left\{ \frac{(\nu-\ell)(\nu-\ell+1)\,\cdots\,(\nu-1)}{(\nu+\ell)(\nu+\ell-1)\,\cdots\,(\nu+1)} \right\}^{1/2} \qquad (\text{A4})$$

That gives at the first order

for $\ell = 0$ $\quad K(\nu,0) = 1/\Gamma(\nu)\,\nu^{3/2}$

for $\ell = 1$ $\quad K(\nu,1) \simeq (1-\sqrt{|\epsilon|})/\Gamma(\nu)\,\nu^{3/2}$

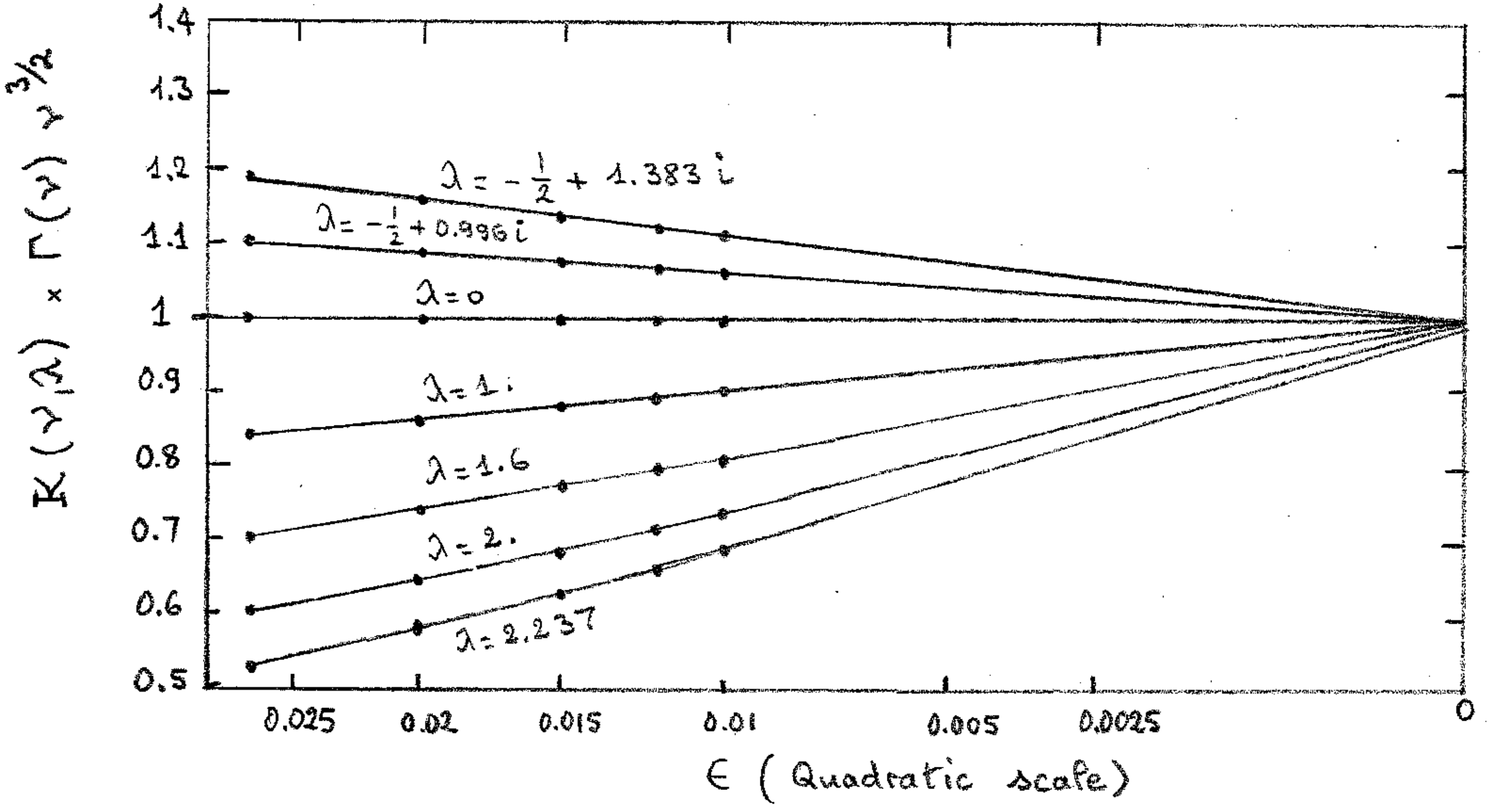
for $\ell = 2$ $\quad K(\nu,2) \simeq (1-3\sqrt{|\epsilon|})/\Gamma(\nu)\,\nu^{3/2}$

$(\,\epsilon = -\frac{1}{\nu^2}\,)$

In the purpose to make dissapear the behaviour in $\sqrt{|\epsilon|}$ we shall use a quadratic scale . On a similar way to Appendix 1 we built a programme for $K(\nu,\lambda)$. On figure A*3 we see that for any λ real or $\lambda = -\frac{1}{2} + i\tilde{\lambda}$ $K(\nu,\lambda)$ is at the first order :

$$K(\nu,\lambda) \simeq \frac{1}{\Gamma(\nu)\,\nu^{3/2}} \left(1 + \beta(\lambda)\sqrt{|\epsilon|} \right) \qquad (\text{A5})$$

****


$K(\nu,\lambda) \times \Gamma(\nu)\, \nu^{3/2}$
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
$\lambda = -\frac{1}{2} + 1.383\, i$
$\lambda = -\frac{1}{2} + 0.996\, i$
$\lambda = 0$
$\lambda = 1.$
$\lambda = 1.6$
$\lambda = 2.$
$\lambda = 2.237$
0.025
0.02
0.015
0.01
0.005
0.0025
0
ϵ (Quadratic scale)

A*3

Appendix 3

The $\underset{\sim}{\mathcal{R}}$ matrix is real and symmetric

We are considering the transformation from $\underset{\sim}{R}$ to $\underset{\sim}{\mathcal{R}}$.

$$\underset{\sim}{F}(\underset{\sim}{R}, r) \sim \left\{ s + c\, \underset{\sim}{R} \right\} \qquad (\text{A6})$$

where $s = \frac{1}{\sqrt{k}} \sin(x)$, $c = \frac{1}{\sqrt{k}} \cos(x)$

X is defined in (2.17).

For the three degenerate channels let's define one coulomb phase only i.e.

$$\left.\begin{array}{lll} s'_1 = s_1 , & c'_1 = c_1 & \\ s'_i = s_2 , & c'_i = c_2 & \text{for } i=2,3,4 \end{array}\right\} \qquad (\text{A7})$$

Then we define

$$\underset{\sim}{F}(\underset{\sim}{R}', r) \sim \left\{ s' + c'\, \underset{\sim}{R}' \right\} \qquad (\text{A8})$$

We have

$$\left.\begin{array}{l} s = s' \cos\varphi + c' \sin\varphi \\ c = c' \cos\varphi - s' \sin\varphi \end{array}\right\} \qquad (\text{A9})$$

φ is the phase difference

$$\underset{\sim}{R}' = (\sin\varphi + \cos\varphi\, \underset{\sim}{R})(\cos\varphi - \sin\varphi\, \underset{\sim}{R})^{-1} \qquad (\text{A10})$$

Let's prove that $\underset{\sim}{R}'$ is symmetric

$$\left.\begin{aligned} \underset{\sim}{R}^T &= \underset{\sim}{R} \\ \underset{\sim}{R}^T(\cos^2\varphi + \sin^2\varphi) &= (\cos^2\varphi + \sin^2\varphi)\,\underset{\sim}{R} \end{aligned}\right\} \quad (\text{A11})$$

This gives

$$\underset{\sim}{R}^T \cos^2\varphi - \sin^2\varphi\, \underset{\sim}{R} = \cos^2\varphi\, \underset{\sim}{R} - \underset{\sim}{R}^T \sin^2\varphi \qquad (\text{A12})$$

By adding to each side $\sin\varphi\cos\varphi - \underset{\sim}{R}^T \cos\varphi \sin\varphi\, \underset{\sim}{R}$ we obtain

$$(\sin\varphi + \underset{\sim}{R}^T\cos\varphi)(\cos\varphi - \sin\varphi\, \underset{\sim}{R}) = (\cos\varphi - \underset{\sim}{R}^T \sin\varphi)(\sin\varphi + \cos\varphi\, \underset{\sim}{R}) \qquad (\text{A13})$$

Finally we have

$$(\cos\varphi - \underset{\sim}{R}^T\sin\varphi)^{-1}(\sin\varphi + \underset{\sim}{R}^T\cos\varphi) = (\sin\varphi + \cos\varphi\, \underset{\sim}{R})(\cos\varphi - \sin\varphi\, \underset{\sim}{R})^{-1}$$

$$\underset{\sim}{R}'^T = \underset{\sim}{R}' \qquad (\text{A14})$$

Due to the properties of s' and c' $\underset{\sim}{O}$ commute with them.

We define

$$\underset{\sim}{G}(\underset{\sim}{R}',r) = \underset{\sim}{O}^T \underset{\sim}{F}(\underset{\sim}{R}',r) \qquad (A15)$$

we have

$$\underset{\sim}{G}(\underset{\sim}{R}',r) \sim (s' \underset{\sim}{O}^T + c' \underset{\sim}{O}^T \underset{\sim}{R}') \qquad (A16)$$

We have also to define

$$\underset{\sim}{G}(\underset{\sim}{\mathcal{R}}',r) \sim s' + c' \underset{\sim}{\mathcal{R}}' \qquad (A17)$$

we obtain

$$\underset{\sim}{\mathcal{R}}' = \underset{\sim}{O}^T \underset{\sim}{R}' \underset{\sim}{O} \qquad (A18)$$

by consequence we have

$$\underset{\sim}{\mathcal{R}}'^T = \underset{\sim}{\mathcal{R}}' \qquad (A19)$$

Between s^*, c^* and s', c' there is aphase difference as between s, c and s', c'. We can deduce that $\underset{\sim}{\mathcal{R}}$ is symmetric because $\underset{\sim}{\mathcal{R}}'$ is symmetric. $\underset{\sim}{\mathcal{R}}$ is also real because all the transformations used were real.

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