AN INVESTIGATION OF KAONIC ATOMS AND MOLECULES

BY

HABATWA VINCENT MWEENE

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Department Of Physics
University Of Surrey
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Dedication

This thesis is dedicated to the memory of my Father, to my Mother, and to the rest of the family, who gave, but waited patiently.
Acknowledgements

I would first and foremost like to thank my supervisor Prof. D. F. Jackson for her patient, understanding, cheerful and knowledgeable guidance. Without a lot of others, this thesis would have been greatly delayed; my profound thanks to Dr M. Harston, Dr M. Yahiro, Dr M. Kamimura, Dr C. Batty, Dr M. Turner, Dr R. Barrett, Dr J. Tostevin, Prof. R Johnson, Mrs J. Hilton and Mr D. Munro. Thanks also go to the Computing Unit, and to the cheerful ladies of the Physics Dept., particularly Mrs L. McCormick. And last, but not least, I wish to record my gratitude to my sponsors, the EDF.
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SECTION I

AN INVESTIGATION OF STRONG-INTERACTION ABSORPTION IN KAONIC-ATOM CASCADE CALCULATIONS
ABSTRACT

Computer programs for simulating the kaonic-atom cascade process require the rates for strong-interaction absorption as well as for radiative and Auger transitions. Due to difficulties in computing the absorption rates, it has been standard practice to only approximately allow for them. In this section of the thesis, the effects of this procedure on the cascade results are investigated. As the approximate methods used heretofore are based on perturbation theory, this approximation is investigated first. A method of computing the widths to second-order in this framework is devised, but perturbation theory is still found to be inadequate. The black-sphere model is more successful, and by using extrapolation to obtain those widths which this model does not directly give, the absorption rates for all states appearing in the cascade calculation are fed in. On the way, the experimentally-observed relationship between the strong-interaction shift and the width in kaonic atoms is theoretically justified. The X-ray intensities from the cascade calculation are found to be negligibly improved by the comprehensive treatment of absorption. It is found that comparing absolute experimental and theoretical intensities is less successful than comparing relative intensities. The conclusion is drawn that previously used methods of dealing with strong-interaction absorption are sufficiently accurate.
In common with other negatively-charged "extraordinary" particles (muons, pions, antiprotons and sigma hyperons), the K$^-$ meson can be captured into orbit about an atomic nucleus to form an "exotic" atom. This was predicted in 1947 by Fermi and Teller [1] and was confirmed for kaons in 1967 [2]. The exotic system is bound mainly by the Coulomb attraction, but since the kaon is a hadron, is also subject to the strong interaction. The strong interaction shifts the binding energies of the states, but more importantly, it is absorptive and draws the kaon into the nucleus to destruction. In consequence of this absorption, de-excitation X rays are increasingly attenuated as the kaon becomes more and more tightly bound, until at last they are extinguished. The study of this process has in the past been stimulated by a hope, originally raised by Jones [3] and subsequently emphasised by Wilkinson [4,5], that absorption could illuminate the distribution of matter in the nuclear surface. Another gain would be increased understanding of the kaon-nucleon strong potential.

On first capture about a nucleus, the kaon is in a state corresponding to principle quantum number $n \approx 60 - 100$, and subsequently cascades to lower- $n$ levels. However, the processes by which capture occurs and by which de-excitation to lower levels
happens are complex and not easily quantified. Reviews of the subject have been written by Backenstoss [6], Burhop [7] and Kim [8]. To achieve an accurate theoretical description, treatment of the kaonic atom is usually considered only for those orbits contained within the electronic K shell. This limit corresponds to $n = 31$.

Simulating the de-excitation cascade by computer is the main way to study the exotic atom. Details of the procedure have been comprehensively described by Turner [9]. The calculation requires the evaluation of X-ray, Auger and strong-absorption transition rates for all states involved in the cascade. The Auger and radiative rates have received much attention and are believed to be sufficiently accurate for all exotic atoms [10-15]. In principle the absorption rate is also accurately obtainable from numerical solution of the Klein-Gordon equation with the strong-interaction potential included. However, the cascade calculation is intrinsically lengthy and admits only relatively fast methods of computing transition rates. For this reason, an approximate formula by West [16] which relates all strong-absorption widths belonging to the same value of $n$ to one experimentally-known value has found useful application in cascade calculations [9,17]. Otherwise, strong-interaction absorption has been neglected altogether [10].

It is not clear whether West's formula is adapted to the case of kaonic atoms. It is implicitly founded on first-order perturbation theory and therefore depends for its success on whether the system is amenable to such a treatment in the first
place. Although an improved version of West's formula \cite{18} has been applied successfully to pionic atoms, the strong interaction is much stronger for kaons than for pions and this raises the possibility that the kaonic-atom system may be too strongly perturbed for proper application of perturbation theory.

The main objective of this investigation is to determine the effect on the accuracy of cascade calculations of only allowing approximately for the absorption width. To this end, the accuracy of perturbation theory in predicting strong-interaction transition rates is first investigated; a conclusion can thereby be drawn as to the validity of West's formula. The use of West's formula presupposes that the cascade process preferentially populates circular-orbit states \cite{19-21}. This belief is reflected in the practice of inserting into cascade calculations only widths corresponding to such states, even though the values of elliptical-orbit-state widths may be large. This study should test the validity of this practice.

The study of the aims occupies three chapters altogether. Chapter 2 contains the investigation of perturbation theory for different sets of parameters in the optical potential representing the strong interaction. Perturbation theory proves inadequate, and inconsequence, another method for calculating widths, the black-sphere model, is presented in Chapter 3. Finally, cascade calculations for a variety of kaonic-atom systems are reported in Chapter 4. Two sets of calculations are performed in each case; on the one hand, the old method of using West's formula to generate only a few widths is employed, and on the other hand the width
for every state that participates in the calculation is supplied. The results of this comparison are presented in the same chapter, as are a few comments.

Before proceeding it is necessary to mention the form in which the experimental data appear. They come in the form of X-ray intensities from which are deduced energy shifts and level broadenings due to the strong interaction, as well as the relative yield of X rays for the lowest two circular-width states observed to take part in the cascade. Only one level broadening is directly measurable - that for the last state to which X rays are observed. If desired, the yield can be converted to the width for the next-to-last circular-orbit state. These details are reviewed by Batty [22-25].

It should be mentioned that since they are connected by the Uncertainty Principle, the width and the transition rate are equivalent, and can be used interchangeably at pleasure.
CHAPTER TWO - ABSORPTION WIDTHS BY PERTURBATION THEORY

SECTION 2.1 - INTRODUCTION

Since the Coulomb attraction between the $K^-$ meson and the nuclear protons is mainly responsible for the binding, the strong interaction can be treated as a perturbation on the kaonic atom. The kaon being spinless, the unperturbed wavefunctions are solutions of the Klein-Gordon equation. Usually, perturbation theory is only useful if the first-order term alone yields sufficiently accurate widths.

SECTION 2.2 - THE STRONG-INTERACTION POTENTIAL

The strong interaction is represented by the optical potential [26-30]

$$V_s = -\frac{2\pi \hbar^2}{\mu} \left(1 + \frac{m_K}{m_N}\right) \left(a_n n_n(r) + a_p p_p(r)\right), \quad (2.1)$$

where

$\mu$ is the kaon-nucleus reduced mass,

$m_k$ is the kaon mass,
\( m_N \) is the nucleon mass,

\( a_n \) is the complex effective scattering length for kaon-neutron scattering,

\( a_p \) is the complex effective scattering length for kaon-proton scattering,

\( \rho_n(r) \) is the neutron-matter density distribution,

\( \rho_p(r) \) is the proton-matter density distribution,

and

\( \hbar \) is Planck's constant.

In first-order perturbation theory, the real part of \( V_s \) is responsible for the shift in the binding energy from the Coulombic value while the imaginary part accounts for the level broadening. What the exact magnitudes of the shift and width are obviously depends on the values of \( a_n \) and \( a_p \). Ideally, the scattering lengths should derive independently from scattering or other data but should reproduce the measured shifts and widths. A straightforward use of the scattering lengths in this way fails to achieve this [31]. Thus, a more practical approach is to obtain them phenomenologically by fitting the shift, yield and width data by numerically integrating the Klein-Gordon equation. For comparison, three sets of scattering lengths are used in this work. Set I is due to a phenomenological analysis of all known shifts, widths and yields by Batty [32]; this set is

\[
\begin{align*}
    a_n &= (0.07 + i0.99) \text{ F}, \\
    a_p &= (0.63 + i0.65) \text{ F}.
\end{align*}
\]
Set II is due to a semi-phenomenological analysis of the data. Deloff [31] has shown that the strength of the optical potential is a non-linear function of the free $K^-p$ and $K^-n$ scattering lengths $a_p$ and $a_n$. According to the analysis,

$$ V_s = -\frac{2m_h}{\mu} (1 + m_K/m_N) \left[ \frac{a_p}{1 + a_p/bq} \rho_p(r) + \frac{a_n}{1 + a_n/bq} \rho_n(r) \right], \quad (2.3) $$

where $bq$ is the parameter to be adjusted to bring about agreement with the data. A chi-squared search for the value of $bq$ has been performed by Batty [32]. The best results have been obtained from the scattering lengths of Martin [33], which are

$$ a_n = (0.35 + i0.66) \text{ F}, \quad (2.4a) $$

and

$$ a_p = (-0.66 + i0.71) \text{ F}, \quad (2.4b) $$

with a corresponding value $bq = 1.12$. Thus, the coefficients of $\rho_p$ and $\rho_n$ in (2.3) are

$$ a_n' = (0.41 + i0.32) \text{ F}, \quad (2.5a) $$

and

$$ a_p' = (0.31 + i1.24) \text{ F}. \quad (2.5b) $$

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Set III is due to Kim [34], and is independent of the shift and width data. It is due to a phenomenological analysis of six reactions of the $K^-$ and the proton in the framework of Dalitz-Tuan reaction theory [35] to obtain the quantities $A_0$ and $A_1$. These are the complex scattering lengths in the $I = 0$ and $I = 1$ isospin channels respectively, in terms of which the low-energy KN scattering lengths can be parametrized at threshold. In the low-energy limit, $a_n$ and $a_p$ are given by

$$a_n = A_1,$$  \hspace{1cm} (2.6a)  
and

$$a_p = (A_0 + A_1)/2.$$  \hspace{1cm} (2.6b)

Kim's values for $A_0$ and $A_1$ then give

$$a_n = (-0.003+i0.688) \, F,$$  \hspace{1cm} (2.7a)  
and

$$a_p = (-0.839+i0.705) \, F.$$  \hspace{1cm} (2.7b)

It is a customary to take for the matter densities $\rho_n$ and $\rho_p$ the Wood-Saxon form, with parameters obtained from electron-scattering experiments [36]:

$$\rho_p(r) = (Z/A)\rho_0/(1 + \exp(4in3(r-c)/t)),$$  \hspace{1cm} (2.8)  
and

$$\rho_n(r) = (N/A)\rho_0/(1 + \exp(4in3(r-c)/t)).$$  \hspace{1cm} (2.9)
where $Z, N,$ and $A$ are the proton, neutron and mass numbers of the nucleus; the other parameters are

$$c = 1.07A^{1/3} \text{ F.}$$  \hspace{1cm} (2.10)

and

$$t = 2.42 \text{ F.}$$  \hspace{1cm} (2.11)

and

$$\rho_0 = (A/4\pi) \left[ \int_0^{\infty} dr \frac{r^2}{(1 + \exp(4ln3(r-c)/t))} \right]^{-1}$$  \hspace{1cm} (2.12)

The first-order perturbation-theory correction to the energy is given by

$$\Delta E_1 = \int \psi_{n,l}^{*} V_s(r) \psi_{n,l} dr,$$  \hspace{1cm} (2.13)

where $n$ and $l$ are the principal and angular-momentum quantum numbers of the state $\psi$. Since the energy change due to the strong interaction is

$$\Delta E = \epsilon - i\Gamma/2,$$  \hspace{1cm} (2.14)

it follows that the energy shift is

$$\epsilon = \int \psi_{n,l}^{*} V_r \psi_{n,l} dr,$$  \hspace{1cm} (2.15)
and the width is

$$\Gamma = -2\int \psi^*_n,l \psi_{1,n,l} dr,$$  \hspace{1cm} (2.16)

where

$$V_s(r) = V_R(r) + iV_I(r).$$  \hspace{1cm} (2.17)

SECTION 2.3 - THE KAONIC-ATOM WAVEFUNCTION

The wavefunctions used here are solutions of the Klein-Gordon equation for a Coulomb point-potential and are given by [37]

$$\psi_{n,l,m} = C_{n,l}(2\mu Ze^2r/nh^2)^{s+1/2} \exp(-Z\mu e^2r/nh^2)/r$$

$$\times F(-(n-1-1),2s+2,2Z\mu e^2r/nh^2) Y^m_l(\theta,\phi),$$  \hspace{1cm} (2.18)

where

- $F$ is the confluent hypergeometric function,
- $Y^m_l$ is a spherical harmonic,
- $e$ is the elementary unit of charge,
- $m$ is the magnetic quantum number,
- $s = -1/2 + ((1 + 1/2)^2 - Z^2 \alpha^2)^{1/2}$,
\( \alpha \) is the fine-structure constant, \(-e^2/\hbar c\),

\( c \) is the speed of light in vacuo,

and

\[
C_{n,I} = \frac{(2Zue^2/nh^2)^{1/2} [(2s+2)(2s+3) \ldots (2s+2+2(n-1-2))]^{1/2}}{[\Gamma(2s+2)(n-1-1)!(1 + (n-1-1)/(s+1))]^{1/2}},
\]

is the radial normalization factor.

The gamma function \( \Gamma \) in the expression for \( C_{n,I} \) is not to be confused with the width.

SECTION 2.4 - RESULTS

Simpson’s rule was used to evaluate the integrals. The accuracy of the computer program was checked by computing normalization integrals, which was satisfactorily achieved.

Tables 2.1a, 2.2a and 2.3a summarise the theoretical widths from the use of data sets I, II and III respectively. The quantity \( \chi^2 \) in column 5 of each table was computed as is usual from the formula

\[
\chi^2 = ((\Gamma_t - \Gamma_e)/\Delta\Gamma_e)^2,
\]

where \( \Gamma_t \) is the theoretical width from column 4; \( \Gamma_e \) is the experimental value from column 3; and \( \Delta\Gamma_e \) is the experimental uncertainty. Tables 2.1b, 2.2b and 2.3b summarise in turn the contents of Tables 2.1a, 2.2a and 2.3a. The experimental data are from references [2,20,38,39,40-42].
<table>
<thead>
<tr>
<th>NUCLEUS</th>
<th>STATE $(n,J)$</th>
<th>EXPERIMENTAL WIDTH (keV)</th>
<th>THEORETICAL WIDTH (keV)</th>
<th>$\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^4$He$_2$</td>
<td>2,1</td>
<td>0.03±0.03</td>
<td>0.003</td>
<td>0.84</td>
</tr>
<tr>
<td>$^7$Li$_3$</td>
<td>2,1</td>
<td>0.055±0.029</td>
<td>0.059</td>
<td>0.018</td>
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<tr>
<td>$^9$Be$_4$</td>
<td>2,1</td>
<td>0.172±0.058</td>
<td>0.345</td>
<td>8.86</td>
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<tr>
<td>$^{10}$B$_5$</td>
<td>2,1</td>
<td>0.810±0.100</td>
<td>1.14</td>
<td>10.9</td>
</tr>
<tr>
<td>$^{11}$B$_5$</td>
<td>2,1</td>
<td>0.700±0.080</td>
<td>1.34</td>
<td>73.7</td>
</tr>
<tr>
<td>$^{12}$C$_6$</td>
<td>2,1</td>
<td>1.730±0.150</td>
<td>3.51</td>
<td>141.</td>
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<tr>
<td>$^{16}$O$_8$</td>
<td>3,2</td>
<td>0.017±0.014</td>
<td>0.012</td>
<td>0.14</td>
</tr>
<tr>
<td>$^{24}$Mg$_{12}$</td>
<td>3,2</td>
<td>0.214±0.015</td>
<td>0.332</td>
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<td>$^{27}$Al$_{13}$</td>
<td>3,2</td>
<td>0.490±0.160</td>
<td>0.685</td>
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<tr>
<td>$^{28}$Si$_{14}$</td>
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<td>0.810±0.12</td>
<td>1.15</td>
<td>8.25</td>
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<td>$^{31}$P$_{15}$</td>
<td>3,2</td>
<td>1.440±0.120</td>
<td>2.133</td>
<td>33.37</td>
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<td>$^{32}$S$_{16}$</td>
<td>3,2</td>
<td>1.96±0.17</td>
<td>3.34</td>
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<td>$^{35.5}$Cl$_{17}$</td>
<td>3,2</td>
<td>3.80±1.0</td>
<td>5.84</td>
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<td>$^{59}$Co$_{27}$</td>
<td>4,3</td>
<td>0.64±0.25</td>
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<td>2.0</td>
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<tr>
<td>$^{58}$Ni$_{28}$</td>
<td>4,3</td>
<td>0.59±0.21</td>
<td>1.26</td>
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<td>$^{63}$Cu$_{29}$</td>
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<td>1.650±0.72</td>
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<td>$^{107}$Ag$_{47}$</td>
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<td>1.54±0.58</td>
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<td>$^{114}$Cd$_{48}$</td>
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<td>2.01±0.44</td>
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<td>$^{115}$In$_{49}$</td>
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<td>2.38±0.57</td>
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<td>$^{120}$Sn$_{50}$</td>
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<td>3.18±0.64</td>
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Table 2.1a: continued on next page
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<th>STATE (n,i)</th>
<th>EXPERIMENTAL WIDTH (keV)</th>
<th>THEORETICAL WIDTH (keV)</th>
<th>$\chi^2$</th>
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<td>$^{165}<em>{\text{Ho}}</em>{67}$</td>
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<td>2.14±0.31</td>
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<td>$^{181}<em>{\text{Ta}}</em>{73}$</td>
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<td>3.76±1.15</td>
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<td>0.37±0.15</td>
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<td>$^{238}<em>{\text{U}}</em>{92}$</td>
<td>7,6</td>
<td>1.50±0.75</td>
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Table 2.1a continued

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<th>STATE (n,i)</th>
<th>NUMBER OF POINTS</th>
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<tr>
<td>2,1</td>
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<td>225.3</td>
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<td>3,2</td>
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<td>628.7</td>
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<td>5,4</td>
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<td>6,5</td>
<td>3</td>
<td>9.7</td>
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<td>7,6</td>
<td>2</td>
<td>1.42</td>
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<td>TOTAL</td>
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Table 2.1b
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<th>EXPERIMENTAL WIDTH (keV)</th>
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<td>0.003</td>
<td>0.81</td>
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<td>0.64±0.25</td>
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<td>2.39±0.30</td>
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<td>$^{238}\text{U}_{92}$</td>
<td>7,6</td>
<td>1.50±0.75</td>
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<td>0.57</td>
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Table 2.3a continued

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Table 2.3b
SECTION 2.5 - ANALYSIS OF RESULTS

It is clear at once that for the low-lying atomic levels, perturbation theory is inadequate. For all sets of data, the value of $\chi^2$-per-point is too high for the levels $(n,l) = (2,1)$ and $(3,2)$. However, agreement is reasonable and even good for the remaining levels. The best overall results are given by Kim's scattering lengths. As these scattering lengths are independent of the data, a hope is raised that physics has been vindicated; however, a closer scrutiny disappoints this hope. Firstly, it is the other scattering lengths which in an exact treatment reproduce the experimental data [32]. Secondly, the apparent superiority of Kim's parameters is evidently due to the accident that they give the lowest values while perturbation theory over-estimates the widths for low-lying states.

As the agreement of theory and experiment is good for the levels $(n,l) = (4,3), (5,4), (6,5)$ and $(7,6)$, West's formula may confidently be used for those nuclei in which the last X rays observed are to these levels. For these nuclei, $Z$ is relatively high. For nuclei with lower $Z$, improvements to perturbation theory and, by subsequent extension, to West's formula are necessary.

The fact that the failure of perturbation theory is correlated to state indicates that, far from being a well-behaved perturbation, the strong interaction seriously affects the form of the wavefunction in the nuclear region. This distortion operates on the lower atomic levels. Now, as $Z$ is progressively increased,
the atomic level at which strong-interaction absorption extinguishes the X rays is higher and higher, so that when Z is high, the meson hardly reaches the affected levels. Thus, wavefunction distortion is most important in light atoms, as the Tables confirm. Before further discussion of this effect, the second-order correction to the energy is investigated.

SECTION 2.6 - THE SECOND-ORDER CORRECTION

The sum which appears in the expression for the second-order term usually requires too much labour for evaluation. Fortunately, in the current case, some of the approximations made about the optical potential permit the expression of this sum as a function of the first-order term. It is important to gauge the magnitude of the second-order term because the distortion of the wavefunction is thereby established, or discounted, as the source of the disagreement between theory and experiment.

The second-order correction to the energy is

\[ \Delta E_2 = \sum_{n' \neq n} \langle n | V_S | n' \rangle \langle n' | V_S | n \rangle / (E_n - E_{n'}) \]  

(2.20)

with kets and bras used for convenience. The angular-momentum quantum numbers \( l \) and \( m \) are omitted because \( V_S \) has been chosen to be spherically symmetric and the orthogonality of the spherical harmonics ensures that \( l' = l \) and \( m' = m \).

Using eq. (2.17) in eq. (2.20) leads to
\[ \Delta E_2 = \sum_{n \neq n'} \left[ \langle n | V_R | n' \rangle \langle n' | V_R | n \rangle - \langle n | V_I | n' \rangle \langle n' | V_I | n \rangle \right] (E_n - E_{n'}). \]

\[ + 2i \sum_{n \neq n'} \langle n | V_R | n' \rangle \langle n' | V_I | n \rangle (E_n - E_{n'}). \]  

(2.21)

To arrive at (2.21) from (2.20), the equalities

\[ \langle n | V_R | n' \rangle = \langle n' | V_R | n \rangle \]

and

\[ \langle n | V_I | n' \rangle = \langle n' | V_I | n \rangle \]

which hold for real wavefunctions and Hermitian operators have been used.

Up to second order, the shift and width are

\[ \epsilon = \langle n | V_R | n \rangle + \sum_{n \neq n'} \frac{\left[ \langle n | V_R | n' \rangle \langle n' | V_R | n \rangle - \langle n | V_I | n' \rangle \langle n' | V_I | n \rangle \right]}{E_n - E_{n'}} \]  

(2.22a)

and

\[ \Gamma = -2 \langle n | V_I | n \rangle - 4 \sum_{n \neq n'} \langle n | V_R | n' \rangle \langle n' | V_I | n \rangle (E_n - E_{n'}). \]  

(2.22b)

Since the matter distributions of protons and neutrons have been taken to be similar, the optical potential may be written as

\[ V = -(2\pi \hbar^2/\mu)(1 + m_K/m_N)(a_{\pi} N/A + a_p Z/A) \rho(r) \]  

(2.23)
where
\[ \rho(r) = \rho_0/(1 + \exp(4in3(r-c)/t)), \]  

(2.24)

so that
\[ V_R = -(2\pi\hbar^2/\mu)(1+m_K/m_N)(N.\text{Real}(a_n) + Z.\text{Real}(a_p))\rho(r)/A \]
\[ = v_R\rho(r), \]  

(2.25)

and
\[ V_I = -(2\pi\hbar^2/\mu)(1+m_K/m_N)(N.\text{Im}(a_n) + Z.\text{Im}(a_p))\rho(r)/A \]
\[ = v_I\rho(r). \]  

(2.26)

Therefore,
\[ \epsilon = v_R \langle n | \rho | n \rangle + (v_R^2 - v_I^2)\sum_{n \neq n'} \langle n | \rho | n' \rangle \langle n' | \rho | n \rangle/(E_n - E_{n'}), \]  

(2.27)

and
\[ \Gamma = -2v_I \langle n | \rho | n \rangle - 4v_R v_I \sum_{n \neq n'} \langle n | \rho | n' \rangle \langle n' | \rho | n \rangle/(E_n - E_{n'}). \]  

(2.28)

Letting
\[ S = \sum_{n \neq n'} \langle n | \rho | n' \rangle^2/(E_n - E_{n'}), \]  

(2.29)

leads to
\[ \epsilon = \nu_R \langle n | \rho | n \rangle + (\nu_R^2 - \nu_I^2)S \]  

(2.30)

and

\[ \Gamma = -2\nu_I \langle n | \rho | n \rangle - 4\nu_R \nu_I S. \]  

(2.31)

By means of the relation \( \epsilon = \pm 0.26\Gamma \), found experimentally to hold regardless of state or nucleus under consideration [30], \( S \) is obtained in terms of \( \Gamma \) alone as

\[ S = (\pm 0.26\Gamma - \nu_R \langle n | \rho | n \rangle)/(\nu_R^2 - \nu_I^2) \]  

(2.32)

The sign of the ratio \( \epsilon/\Gamma \) is determined by that of the shift, which in turn is fixed by the sign of \( Z.\text{Real}(a_p) + N.\text{Real}(a_n) \).

From (2.32) and (2.31), the width is obtained to second order as

\[ \Gamma = (\nu_R^2 + \nu_I^2)\Gamma_1/(\nu_I^2 - \nu_R^2 \pm 1.04\nu_R \nu_I) \]  

(2.33)

where \( \Gamma_1 \) is the first-order width \(-2\nu_I \langle n | \rho | n \rangle \).

The factor

\[ F = (\nu_R^2 + \nu_I^2)/(\nu_I^2 - \nu_R^2 \pm 1.04\nu_R \nu_I) \]  

(2.34)

which adjusts the first-order widths has been calculated and is
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<th>SET II</th>
<th>SET III</th>
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Table 2.4. Values of the correction factor, eq. (2.34) for the three sets of scattering lengths.
shown in Table 2.4 for the three sets of scattering lengths. It is evidently independent of state, but is a function of $Z$ and $N$ through $v_R$ and $v_I$.

A perusal of Table 2.4 shows that the factor $F$ is inadequate to reduce the discrepant lower-level widths to the experimental values. This shows that something more fundamental than the absence of the second-order contribution to the widths listed in Tables 2.1a, 2.2a and 2.3a is responsible for the disagreement. Incidentally, the fact that the parameters of Kim predict shifts of opposite sign from the other two sets is reflected in the sign of $e/r$ and thus in the values of $F$ in Table 2.4.

SECTION 2.7 - STRONG-INTERACTION DISTORTION OF THE WAVEFUNCTION

The effect of the strong interaction on the kaonic-atom wavefunction was first pointed out independently by Seki [43,44] and by Krell [45]. A similar effect had already been observed in studies of pionic atoms [46]. In both cases, the real part of the optical potential is responsible for altering the shape of the wavefunction in the nuclear region. Ericson and Scheck [47] demonstrated this by integrating the Klein-Gordon equation with the imaginary part of the potential set to zero and the real part set to different strengths. The wavefunctions thus obtained were used to perturbatively calculate the shifts, yields and widths. The three quantities proved to be strong functions of the strength of the real part of the optical potential. It was thereby shown that for perturbation theory to perform well, distorted wavefunctions are needed. Since these wavefunctions are not
analytically known, it is not possible to imitate West's reasoning to obtain an analogue to his formula. To obtain them numerically is less laborious than to solve the Klein-Gordon equation for the widths, since the imaginary part of the optical potential is left out, but the whole process is still too time-consuming to be practical.

SECTION 2.8 - FACTORS AFFECTING THE VALUE OF THE WIDTH

Before leaving the perturbation-theory approach, some factors which bear on its success are touched upon.

The width values depend on the half-density radius $c$ and the difussivity parameter $t$ in expresions (2.8) and (2.9). Because kaon absorption occurs in the very periphery of the nucleus, [3,4,48], the width is very sensitive to these parameters. Investigations by Burhop [49], Batty [32], Martin [21] and Backenstoss et. al. [38] have confirmed this fact. This point has not been investigated here, but it is probable that in order to get good widths with undistorted wavefunctions, $c$ and $t$ would have to be separately adjusted for each case. Furthermore, there is little theoretical reason to adjust $c$ and $t$ from their electron-scattering-data values. An early conviction that there is a preponderance of neutrons in the nuclear surface [52,53] has largely been discredited [47,54].

Uncertainties in the form of the strong-interaction potential might introduce discrepancies into theoretical widths. This is unlikely though, owing to the fact that when the free KN
scattering lengths are more rigorously related to the strength of the potential, as Deloff [31] has shown, good agreement of exact theory (numerical integration of the Klein-Gordon equation) with experiment is achieved. Moreover, if the functional form of the optical potential was seriously inappropriate, the phenomenological analysis of Batty [32] would have been less successful. A neglected contribution to the potential is that due to the p-wave interaction, which would be represented by a gradient term. Studies by Backenstoss et al. [38], Ericson and Schöck [47], and Krell [45] have shown that this is indeed negligible.

It is known that two-nucleon absorption of the kaon accounts for 15-20% of the absorption [55]; this would be represented by a term proportional to the square of the matter distribution in the optical potential. From the standpoint of perturbation theory, its inclusion could only aggravate the discrepancy by increasing the theoretical widths.

A complication of a calculation of the width by any method arises from the fact that absorption of kaons on protons is attenuated by the existence of the $Y^*_0$ particle in that channel at an energy lying 31 MeV below the sum of rest-energies of the $K^-$ and the proton. Attempts to tackle this problem are reported in references [56-58].

Other problems relate to the effects of the finite range of the nucleon-meson interaction; nuclear deformation; polarization induced by the $K^-$ meson; and the finiteness of the nuclear charge distribution. With the possible exception of the last one, these
complications are expected to exercise a negligible influence on the widths. To rigorously correct for any of them would require so much calculational labour as to defeat the main objective of this study.
CHAPTER THREE - WIDTHS BY THE BLACK-SPHERE MODEL

SECTION 3.1 - INTRODUCTION

It has been seen in the previous chapter that the kaonic-atom strong interaction is too strong to allow the absorption widths to be calculated by perturbation theory. The very strength of the potential can be exploited to evaluate them by another approach: the black-sphere model. Here, the nucleus is treated as a totally-absorbing sphere which captures all kaons venturing within a certain distance of it. Kaufmann and Pilkuhn [59,60] have based their formulation on the WKB method; it yields values rivalling those from exact treatment in accuracy [32]. The width and the shift are given in closed form, making this a very fast method of computing them, and thus satisfying the main requirement for use in cascade codes.

The main arguments on which the black-sphere treatment hinge are to be sketched later. The final formula for the width is [59,60]:

\[
\Gamma = 0.89\nu_0\theta^{-2},
\]  

(3.1)

where
\[ \nu_0 = -E_n/(n'\pi), \]  
\[ E_n = \mu'(Z\alpha)^2/(2n'^2). \]  

and the Klein-Gordon hydrogenic energy is

The other quantities are

\[ n' = n - (1+1/2) + ((1+1/2)^2 - (Z\alpha)^2)^{1/2}, \]  

\( \alpha \) being the fine-structure constant;

\[ \exp^{-2} = \frac{(n'^2 - \lambda'^2)^{n'+\lambda'}(y/(n'\lambda'))^{2\lambda'} \exp(2Y)}{(Y + \lambda' - y/\lambda')^{2\lambda'} (n' - Y - y/n')^{2n'}}, \]

where

\[ \lambda' = (l(l + 1) - (Z\alpha)^2)^{1/2}, \]  
\[ y = Z\alpha\mu'R, \]  
\[ Y = (\lambda' - 2y + (y/n')^2)^{1/2}, \]  
\[ \mu' = \mu/(1 + (Z\alpha/n')^2)^{1/2}; \]

and \( \mu \) is the kaon-nucleus reduced mass, while \( R = 1.42A^{1/3}F \) is the "effective nuclear radius for absorption."

SECTION 3.2 - THE BLACK-SPHERE APPROXIMATION

The strong-interaction potential does not appear explicitly in this model. The reason is that since the potential is both
attractive and absorptive, the absorption probability is independent of the details of the nuclear interior. Once the hadron ventures into the region of strong interaction, it is trapped by the attraction of the potential and annihilation is inevitable. Due to the fact that to a very good approximation the strong interaction has the same functional dependence on $r$ (where $r$ is the distance of the kaon from the centre of the nucleus) as the matter density, whose boundary is abrupt, this region is very clearly defined. The precise value of the absorption probability is decided by the probability that the kaon is at the critical radius $R$, which in turn is determined by the wavefunction beyond this radial distance. Beyond this distance, the potential is Coulombic, and so is the wavefunction. The effect of the strong interaction appears suddenly at the critical radius. Thus, indeed, the nucleus can be replaced by a sphere the details of whose interior are irrelevant, whose role is to annihilate kaons which find themselves at the critical radius mainly because of the Coulomb attraction.

The black-sphere model has some limitations which mean that it will not give widths for arbitrary values of $n$ and $l$. These can be largely overcome by extrapolation methods to be explained later. An outline of the method is now given.

SECTION 3.3 - OUTLINE OF THE BLACK-SPHERE TREATMENT

Outside the nucleus, the kaon moves in a potential which is in Fig. 3.1. In relativistic units $\hbar=c=1$, this potential is
Fig. 3.1: Plot of $l>0$ effective potential seen by the kaon.
\[ V_{\text{eff}} = -2\alpha/r + I(1+1)/(2\mu r^2). \] (3.10)

The regions I, II, III and IV defined in Fig. 3.1 have different forms for the wavefunction. The expressions are given in Merzbacher's "Quantum Mechanics" [61] in the chapter on the WKB method. In region IV, which is the nuclear interior, a boundary condition describes the wavefunction by summarising the effect of the strong interaction. Since the kaon has to penetrate beyond \( R \) to suffer its fate, the assumption is made that this is equivalent to a classically-allowed domain just inside the nucleus, with the wavefunction

\[ \varphi_{IV} = k^{-1/2} [A \exp(i\int_{R}^{r} kdr) + B \exp(-i\int_{R}^{r} kdr)], \] (3.11)

far from the turning point \( r_1 \).

The other solutions, far from the turning points, are

\[ \varphi_{I} = k^{-1/2} \exp(-\int_{r_2}^{r} kdr) \quad \text{for} \quad r > r_2 \] (3.12)

and

\[ \varphi_{II} = k^{-1/2} [G \exp(-i\int_{r_1}^{r} kdr) + F \exp(i\int_{r_1}^{r} kdr)], \quad \text{for} \quad r_1 < r < r_2, \] (3.13)

where \( k = \sqrt{[2\mu(E - V_{\text{eff}})]^{1/2}} \), \( k = ik \), and \( E \) is the energy.

In region III, classically forbidden, the wavefunction is a sum of increasing and decreasing exponential forms, but the explicit formula is not needed.

In expression (3.11), the first term represents an outward-propagating wave and the second an inward wave. As the
nucleus is absorptive, it is taken that $A = \beta B$, where $\beta = 0$ if absorption is total. With all necessary expressions at hand, the treatment proceeds by adhering closely to the development given by Merzbacher. The seemingly-arbitrary coefficient $\beta$ is ultimately fixed by relating it to the experimental finding $\epsilon = 0.26\Gamma$, which has already been exploited in Chapter 2.

SECTION 3.4 - THE RATIO OF THE SHIFT TO THE WIDTH

It is instructive to digress and give a justification of the constancy of the ratio $\epsilon/\Gamma$. If it is supposed that first-order perturbation theory with distorted wavefunctions gives accurate shifts and widths, the expressions for these quantities are

$$\epsilon = v_R \langle \varphi_d | \rho(r) | \varphi_d \rangle$$

(3.15)

and

$$\Gamma = -2v_I \langle \varphi_d | \rho(r) | \varphi_d \rangle$$

(3.16)

where $v_R$, $v_I$ and $\rho$ are defined in Chapter 2.

Thus,

$$|\epsilon/\Gamma| = \left| v_R / (-2v_I) \right|$$

$$= \frac{(1/2)(\text{Re}(a_p^* N/Z \text{Re}(a_n)) + (N/Z)\text{Im}(a_p^*) + (N/Z)\text{Im}(a_n))}{(\text{Im}(a_p^*) (N/Z)\text{Im}(a_n))}.$$  

(3.17)
A quick check shows that for the parameters of set I, this ratio is 0.21 for $N/Z = 1$ and is 0.17 for $N/Z = 1.5$.

For parameter-set II, the ratio is 0.23 for $N/Z = 1$ and is 0.27 for $N/Z = 1.5$.

Finally, for set III, the ratio is 0.30 for $N/Z = 1$ and is 0.24 for $N/Z = 1.5$.

These values are in qualitative agreement with the experimental one.

SECTION 3.5 - LIMITATIONS OF THE BLACK SPHERE MODEL

Limitations to the black-sphere approach have already been alluded at. The method breaks down for certain values of $n$ and $l$. In particular, it does not give widths for $l = 0$, since there is no centrifugal contribution to the potential, and the inner turning point, pivotal to the treatment, does not exist. Generally, it fails whenever this turning point is smaller than $R$. Mathematically, this failure is manifested by the argument of one of the square roots in the expression for $\Gamma$ becoming negative. For all experimentally-measured widths, the inner turning point is well beyond the critical radius $R$.

SECTION 3.6 RESULTS

Table 3.1 shows how black-sphere-model widths compare with the experimental values. This table is to be contrasted with Tables 2.1, 2.2 and 2.3. The black-sphere-model widths are very satisfactory.
<table>
<thead>
<tr>
<th>NUCLEUS</th>
<th>STATE ((n,l))</th>
<th>EXPERIMENTAL WIDTH (keV)</th>
<th>THEORETICAL WIDTH (keV)</th>
<th>(\chi^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^4)He(_2)</td>
<td>2,1</td>
<td>0.03±0.03</td>
<td>0.004</td>
<td>0.8</td>
</tr>
<tr>
<td>(^7)Li(_3)</td>
<td>2,1</td>
<td>0.055±0.029</td>
<td>0.051</td>
<td>0.019</td>
</tr>
<tr>
<td>(^9)Be(_4)</td>
<td>2,1</td>
<td>0.172±0.058</td>
<td>0.250</td>
<td>1.81</td>
</tr>
<tr>
<td>(^{10})B(_5)</td>
<td>2,1</td>
<td>0.810±0.100</td>
<td>0.757</td>
<td>0.28</td>
</tr>
<tr>
<td>(^{11})B(_6)</td>
<td>2,1</td>
<td>0.700±0.080</td>
<td>0.831</td>
<td>2.68</td>
</tr>
<tr>
<td>(^{12})C(_7)</td>
<td>2,1</td>
<td>1.730±0.150</td>
<td>1.981</td>
<td>2.8</td>
</tr>
<tr>
<td>(^{16})O(_8)</td>
<td>3,2</td>
<td>0.017±0.014</td>
<td>0.0090</td>
<td>0.33</td>
</tr>
<tr>
<td>(^{24})Mg(_{12})</td>
<td>3,2</td>
<td>0.214±0.015</td>
<td>0.225</td>
<td>0.538</td>
</tr>
<tr>
<td>(^{27})Al(_{13})</td>
<td>3,2</td>
<td>0.490±0.160</td>
<td>0.438</td>
<td>0.106</td>
</tr>
<tr>
<td>(^{28})Si(_{14})</td>
<td>3,2</td>
<td>0.810±0.12</td>
<td>0.723</td>
<td>0.52</td>
</tr>
<tr>
<td>(^{31})P(_{15})</td>
<td>3,2</td>
<td>1.440±0.120</td>
<td>1.257</td>
<td>2.33</td>
</tr>
<tr>
<td>(^{32})S(_{16})</td>
<td>3,2</td>
<td>1.96±0.17</td>
<td>1.916</td>
<td>0.067</td>
</tr>
<tr>
<td>(^{35.5})Cl(_{17})</td>
<td>3,2</td>
<td>3.80±1.0</td>
<td>3.12</td>
<td>0.46</td>
</tr>
<tr>
<td>(^{59})Co(_{27})</td>
<td>4,3</td>
<td>0.64±0.25</td>
<td>0.73</td>
<td>0.13</td>
</tr>
<tr>
<td>(^{58})Ni(_{28})</td>
<td>4,3</td>
<td>0.59±0.21</td>
<td>0.923</td>
<td>2.51</td>
</tr>
<tr>
<td>(^{63})Cu(_{29})</td>
<td>4,3</td>
<td>1.650±0.72</td>
<td>1.380</td>
<td>0.14</td>
</tr>
<tr>
<td>(^{107})Ag(_{47})</td>
<td>5,4</td>
<td>1.54±0.58</td>
<td>1.53</td>
<td>0.00030</td>
</tr>
<tr>
<td>(^{114})Cd(_{48})</td>
<td>5,4</td>
<td>2.01±0.44</td>
<td>2.08</td>
<td>0.025</td>
</tr>
<tr>
<td>(^{115})In(_{49})</td>
<td>5,4</td>
<td>2.38±0.57</td>
<td>2.51</td>
<td>0.052</td>
</tr>
</tbody>
</table>

Table 3.1a; continued on next page
<table>
<thead>
<tr>
<th>NUCLEUS</th>
<th>STATE (n,l)</th>
<th>EXPERIMENTAL WIDTH (keV)</th>
<th>THEORETICAL WIDTH (keV)</th>
<th>$\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{120}\text{Sn}_{50}$</td>
<td>5,4</td>
<td>3.18±0.64</td>
<td>3.22</td>
<td>0.0039</td>
</tr>
<tr>
<td>$^{165}\text{Ho}_{67}$</td>
<td>6,5</td>
<td>2.14±0.31</td>
<td>1.40</td>
<td>5.70</td>
</tr>
<tr>
<td>$^{174}\text{Y}_{70}$</td>
<td>6,5</td>
<td>2.39±0.30</td>
<td>2.40</td>
<td>0.0011</td>
</tr>
<tr>
<td>$^{181}\text{Ta}_{73}$</td>
<td>6,5</td>
<td>3.76±1.15</td>
<td>3.85</td>
<td>0.0061</td>
</tr>
<tr>
<td>$^{208}\text{Pb}_{82}$</td>
<td>7,6</td>
<td>0.37±0.15</td>
<td>0.34</td>
<td>0.04</td>
</tr>
<tr>
<td>$^{238}\text{U}_{92}$</td>
<td>7,6</td>
<td>1.50±0.75</td>
<td>1.80</td>
<td>0.16</td>
</tr>
</tbody>
</table>

Table 3.1a continued

<table>
<thead>
<tr>
<th>STATE (n,l)</th>
<th>NUMBER OF POINTS</th>
<th>$\chi^2$</th>
<th>$\chi^2$ PER DATA POINT</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,1</td>
<td>6</td>
<td>8.39</td>
<td>1.4</td>
</tr>
<tr>
<td>3,2</td>
<td>13</td>
<td>21.9</td>
<td>1.68</td>
</tr>
<tr>
<td>4,3</td>
<td>4</td>
<td>7.59</td>
<td>1.85</td>
</tr>
<tr>
<td>5,4</td>
<td>4</td>
<td>0.082</td>
<td>0.021</td>
</tr>
<tr>
<td>6,5</td>
<td>3</td>
<td>5.7</td>
<td>1.9</td>
</tr>
<tr>
<td>7,6</td>
<td>2</td>
<td>0.20</td>
<td>0.10</td>
</tr>
<tr>
<td>TOTAL</td>
<td>32</td>
<td>43.9</td>
<td>1.37</td>
</tr>
</tbody>
</table>

Table 3.1b
It is emphasised that the ultimate aim of this project is to perform a cascade calculation without neglecting a single absorption width. Therefore, an extension of the black-sphere model is needed to supply those widths which equation (3.1) does not give.

A plot of \( \ln \Gamma \) against \( n \) for the sequence of states \((n_0^+1,l_0^+1), (n_0^+2,l_0^+2), \ldots \ldots \) where \((n_0,l_0)\) is an arbitrary combination, is shown in Fig. 3.2. The graph exhibits a smooth behaviour which in fact is general to all such curves investigated. This smoothness suggests that extrapolating the curve gives an accurate value for the width for the state \((n_0,l_0)\). Underlying the validity of such a procedure is the knowledge that the width could be found by integrating the Klein-Gordon equation; the failure of the black-sphere model to supply the width is due to accidental shortcomings of the method only.

There is a practical reason for plotting \( \ln \Gamma \) rather than \( \Gamma \) - the width changes by an order of magnitude or more from one level \((n,l)\) to another \((n\pm1,l\pm1)\), so that scaling difficulties would appear if \( \Gamma \) rather than \( \ln \Gamma \) was plotted. This problem is not peculiar to the actual physical plotting, but affects the numerical process as well; it turns out that the shape of the plot of \( \Gamma \) against \( n \) is not as well suited to being approximated by the polynomial least-squares method as is that of \( \ln \Gamma \). Even though the errors committed on getting the value of \( \ln \Gamma(n_0,l_0) \) by extrapolation are amplified on subsequent exponentiation, the \( \ln \Gamma \) plot gives superior results to the \( \Gamma \) graph.

Whenever an argument of one of the various square roots involved in the definition of \( \Gamma \) is negative, the method has broken
Fig. 3.2: A typical plot of $\ln \Gamma$ against $n$.

This graph would be used to obtain $\Gamma(n=4, l=2)$ by extrapolation.

$Z=13$. 

$Z=13$. 
down and extrapolation is invoked. Suppose this happens for the state \((n_0, l_0)\). A sequence of points defining a curve like Fig. 3.2 generated and used to construct a least-squares polynomial to be used for extrapolation. Two methods are available for the extrapolation-proper - either using the least-squares curve directly or differentiating it in order to use the Taylor formula. The first method yields fluctuating results strongly dependent on the degree of polynomial chosen. This is perhaps not surprising, given that the least-squares curve does not guarantee consistent accuracy outside the range of the data points. On the other hand, if the least-squares curve is faithful in the range of the data points, then presumably so too are the derivatives, and the Taylor-expansion method can be expected to give better accuracy.

After some trial and error, 10 was chosen for the degree of the approximating polynomial and 7 for the number of terms in the Taylor expansion.

In Table 3.2 are displayed the results of tests on the accuracy of extrapolation. All the widths featured are available directly from formula (3.1), and therefore afford a convenient means of comparison. The accuracy is seen to be generally acceptable. Nevertheless, a caution needs to be recorded - namely that the choice of the widths used is random, but could well be fortuitous with regard to comparison. There is no guarantee that a different set would not reveal serious inadequacy in the extrapolation procedure or principle. A statement can be made concerning the effect this would have on the cascade calculation.
<table>
<thead>
<tr>
<th>NUCLEUS</th>
<th>STATE</th>
<th>WIDTH (keV)</th>
<th>EXTRAPOLATION</th>
<th>FORMULA (3.1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Z</td>
<td>A</td>
<td>n</td>
<td>l</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>7</td>
<td>2</td>
<td>8.11×10^{-3}</td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>5</td>
<td>4</td>
<td>3.51×10^{-9}</td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>10</td>
<td>3</td>
<td>4.33×10^{-9}</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>10</td>
<td>4</td>
<td>1.62×10^{-19}</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>3</td>
<td>2</td>
<td>5.48×10^{-8}</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>9</td>
<td>5</td>
<td>2.85×10^{-25}</td>
</tr>
<tr>
<td>20</td>
<td>40</td>
<td>4</td>
<td>2</td>
<td>5.40</td>
</tr>
<tr>
<td>20</td>
<td>40</td>
<td>6</td>
<td>2</td>
<td>2.40</td>
</tr>
<tr>
<td>20</td>
<td>40</td>
<td>10</td>
<td>2</td>
<td>0.466</td>
</tr>
</tbody>
</table>

Table 3.2 - Widths by extrapolation and by exact formula
SECTION 3.7 - EFFECTS OF INACCURACIES IN THE WIDTHS ON THE
CASCADE CALCULATION

According to Table 3.1, the width for the most important state, - the circular-orbit one to which the last X-ray transitions are observed - is given accurately. The next-most-important state has $n$ and $l$ values increased by unity and formula (3.1) directly gives its width. The formula also gives the widths directly for slightly elliptical orbits, and probably also for all but the most elliptical ones. As departure from preferential occupation of circular orbits is not expected to be large, a degree of inaccuracy in the widths of very elliptical orbits can be tolerated.

A second factor is that the absorption width changes very rapidly with quantum numbers, as Table 3.3 shows. Thus for most states, it is either negligible or overwhelming with respect to X-ray and Auger transition rates. In the first case its effect on the X-ray intensity is negligible, while in the second, there are no X rays anyway. Again, this means that fairly large errors in the width exert little influence on the cascade calculation.

Despite these considerations, it is wise to change the extrapolation-criterion. To ensure greater accuracy, extrapolation is now called upon whenever the inner turning point is such that $r_1 \leq 2R$. The reason for this is that it is not known if the method breaks down abruptly at $r_1 = R$ or whether the widths become more and more inaccurate as $r_1$ nears $R$; indeed, the second case is more likely. It should be remembered that the wavefunctions used to derive formula (3.1) are defined for regions
Table 3.3 - Change of width with quantum numbers for $Z = 10$ and $A = 20$. Widths calculated by formula (3.1).
"far from the turning points." It is well therefore to ensure that this condition is fulfilled by keeping $R$ far from $r_1$.

In the next chapter, the black-sphere model is used in cascade calculations.
4.1 - INTRODUCTION

It was observed in Chapter 1 that, heretofore, it has been standard practice to employ only a few absorption widths in cascade calculations. Having found a method of calculating accurately any widths which might be required, it is now possible to test the accuracy of this approximation. For this purpose, a cascade code originally written by Turner [9] is used. In this exercise, the original version of the code uses West's formula

\[
\frac{\Gamma(n=N,1)}{\Gamma(n=M,1)} = \frac{(M/N)^{2l+4}}{(N+1)!(M-l-1)!} \frac{(N+1)!(M-l-1)!}{(M+1)!(N-l-1)!}
\]  

(4.1)

to calculate a few more widths from a number supplied either by experiment or by numerical solution of the Klein-Gordon equation. A modified version uses a new routine to obtain all widths by the black-sphere model, as explained in Chapter 3.

4.2 - THE INITIAL POPULATION DISTRIBUTION AND THE REFILLING WIDTH

Of the other quantities entering the cascade calculation, two deserve brief discussion. The initial distribution of kaons in the substates of the starting-value of \( n \) is not known accurately from theory. It is usual to try several distributions and to accept the one which reproduces the measured intensities best. For the general meson-cascade problem, the modified
statistical distribution [9,62-67] and the quadratic [19,68-70] have been used. Sometimes, the device of populating the 1 substates up to a certain limit only has secured the best results [71,72]. In this work, the modified statistical distribution

\[ P(l) \propto (2l + 1)\exp(\alpha l), \]

(4.2)

where \( \alpha \) is a constant, is used.

The second parameter of interest is the rate at which electrons lost from the electronic shells by kaonic Auger transitions are replenished. If electronic-shell refilling is neglected, cascade results do not fit experimental values because then the Auger rates are under-estimated: good accounts of this topic are given by Vogel [70] and Turner [9]. Values of theoretical refilling widths are given in references [73-81]. In this work, values employed by Vogel in calculations on muonic atoms are used.

The kaonic-atom species S and P have been selected for investigation because they have already been treated by Backenstoss et al. [39] "approximately"; thus the value of \( \alpha \) has already been determined. This is a great convenience, because otherwise, a laborious search for this quantity would have to be conducted; as it is the value from [39] is simply adopted. Of course, with the change to the cascade code, new optimum parameters probably obtain - however, to draw the desired conclusions does not require \( \alpha \) or any other phenomenological quantity to have its optimum value. If these parameters are independent, they can be optimised one at a time. This principle
is usually assumed and means that any effects which depend on the absorption widths will be manifested whatever the value of $\alpha$ or the refilling width.

4.3 - RESULTS

The experimental data are derived from references [39] and [72]. The reason for choosing two sets of data is that in the one case [72], the X-ray intensities are absolute, while in the other [39], they are relative.

Tables 4.1 to 4.6 give the comparisons between experimental and theoretical X-ray intensities. In each table, the values in column 3 pertain to the use of West's formula for the absorption widths while those in column 4 relate to the use of the black-sphere model. The values of $\chi^2$ in columns 4 and 6 correspond to the intensities in columns 3 and 5 respectively.

4.4 DISCUSSION AND CONCLUSION

The tables show that the absolute theoretical and experimental intensities do not match while the relative intensities compare satisfactorily except in Table 4.2. This table contains relative intensities for $P$ from Godfrey's data [72] and are too high compared to the theoretical. However, the same transitions yield higher relative intensities according to the data of Backenstoss et al. [39]. If the possibility of systematic experimental error by Godfrey is admitted, it can be
### Table 4.1. Comparison of absolute X-ray intensities for $^{31}\text{P}_{15}$

The number of X rays is for each stopped kaon. West refers to the case where the absorption widths are calculated by West's formula, while B-S refers to the case where the black-sphere model is used. Widths fed in for the levels $(n,l) = (3,2)$ and $(4,3)$ for use in West's formula. Data from ref. [72].

$$\alpha = 0.10; \text{ refilling width} = 0.17 \text{ eV.}$$

<table>
<thead>
<tr>
<th>TRANSITION NO. X RAYS</th>
<th>NO. X RAYS</th>
<th>$\chi^2$</th>
<th>NO. X RAYS $\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n \rightarrow n$</td>
<td>EXPERIMENTAL</td>
<td>WEST WIDTHS</td>
<td>B-S WIDTHS</td>
</tr>
<tr>
<td>5 4</td>
<td>0.31±0.054</td>
<td>0.56</td>
<td>16.4</td>
</tr>
<tr>
<td>4 3</td>
<td>0.076±0.015</td>
<td>0.18</td>
<td>48.1</td>
</tr>
<tr>
<td>6 4</td>
<td>0.024±0.007</td>
<td>0.080</td>
<td>64.0</td>
</tr>
<tr>
<td>7 4</td>
<td>0.012±0.006</td>
<td>0.027</td>
<td>6.3</td>
</tr>
</tbody>
</table>

### Table 4.2. Comparison of relative intensities for $^{31}\text{P}_{15}$

Widths fed in for levels $(n,l) = (3,2)$ and $(4,3)$ for use in West's formula. Data from ref. [72].

$$\alpha = 0.10; \text{ refilling width} = 0.17 \text{ eV.}$$

<table>
<thead>
<tr>
<th>TRANSITION NO. X RAYS</th>
<th>NO. X RAYS</th>
<th>$\chi^2$</th>
<th>NO. X RAYS $\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n \rightarrow n$</td>
<td>EXPERIMENTAL</td>
<td>WEST WIDTHS</td>
<td>B-S WIDTHS</td>
</tr>
<tr>
<td>5 4</td>
<td>100.0±15.8</td>
<td>100.0</td>
<td>0</td>
</tr>
<tr>
<td>4 3</td>
<td>22.7±4.45</td>
<td>32.1</td>
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<tr>
<td>6 4</td>
<td>7.06±2.09</td>
<td>14.3</td>
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<tr>
<td>7 4</td>
<td>3.53±1.79</td>
<td>4.82</td>
<td>0.52</td>
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</table>

56
Table 4.3. Comparison of relative widths for $^{31}P_{15}$.

Widths fed in for levels $(n,l) = (3,2)$ and $(4,3)$ for use in West's formula. Data from ref. [63].

$\alpha = 0.10$; refilling width = 0.17 eV.

<table>
<thead>
<tr>
<th>TRANSITION NO.</th>
<th>X RAYS</th>
<th>EXPERIMENTAL</th>
<th>NO. X RAYS $\chi^2$</th>
<th>WEST WIDTHS</th>
<th>NO. X RAYS $\chi^2$</th>
<th>B-S WIDTHS</th>
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<tr>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>100.0±2.3</td>
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<td>14.24</td>
<td>44.5</td>
<td>14.23</td>
<td>44.3</td>
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<tr>
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<td>99.0±7.8</td>
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<td>1.11</td>
<td>90.9</td>
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<td>3</td>
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<td>TRANSITION $n \rightarrow n$</td>
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<td>NO. X RAYS B-S WIDTHS $\chi^2$</td>
<td></td>
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</tr>
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<td>-------------------------------</td>
<td>-------------------------------</td>
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<tr>
<td>7 6</td>
<td>0.237±0.042</td>
<td>0.346</td>
<td>6.7</td>
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</tr>
<tr>
<td>6 5</td>
<td>0.364±0.055</td>
<td>0.530</td>
<td>9.1</td>
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<tr>
<td>5 4</td>
<td>0.361±0.54</td>
<td>0.631</td>
<td>25.1</td>
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<tr>
<td>9 6</td>
<td>0.008±0.002</td>
<td>0.015</td>
<td>12.3</td>
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<tr>
<td>8 5</td>
<td>0.013±0.002</td>
<td>0.025</td>
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<tr>
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<td>0.015±0.003</td>
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<tr>
<td>9 5</td>
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<td>0.009</td>
<td>9.0</td>
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<td>8 4</td>
<td>0.006±0.002</td>
<td>0.011</td>
<td>6.3</td>
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</tr>
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Table 4.4. Comparison of absolute intensities for $^{32}$S$_{16}$. Widths fed in for levels $(n,l) = (3,2)$ and $(4,3)$ for use in West's formula. Data from ref. [72]. $\alpha = 0.14$; refilling width = 0.225 eV.
<table>
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<tr>
<th>TRANSITION n → n</th>
<th>NO. X RAYS EXPERIMENTAL</th>
<th>NO. X RAYS WEST WIDTHS</th>
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<th>NO. X RAYS B-S WIDTHS</th>
<th>$\chi^2$</th>
</tr>
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<tbody>
<tr>
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<td>66.7±11.2</td>
<td>54.8</td>
<td>1.13</td>
<td>55.2</td>
<td>1.05</td>
</tr>
<tr>
<td>6 5</td>
<td>100±16.9</td>
<td>84.0</td>
<td>0.99</td>
<td>84.5</td>
<td>0.84</td>
</tr>
<tr>
<td>5 4</td>
<td>100±14.9</td>
<td>100.0</td>
<td>0</td>
<td>100.0</td>
<td>0</td>
</tr>
<tr>
<td>4 3</td>
<td>13.1±2.25</td>
<td>24.2</td>
<td>24.3</td>
<td>24.1</td>
<td>23.9</td>
</tr>
<tr>
<td>7 5</td>
<td>11.1±1.69</td>
<td>12.9</td>
<td>1.13</td>
<td>12.9</td>
<td>1.26</td>
</tr>
<tr>
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<td>10.8±1.69</td>
<td>12.5</td>
<td>1.01</td>
<td>12.4</td>
<td>0.90</td>
</tr>
<tr>
<td>9 6</td>
<td>2.22±0.56</td>
<td>2.36</td>
<td>0.063</td>
<td>2.36</td>
<td>0.063</td>
</tr>
<tr>
<td>8 5</td>
<td>3.61±0.56</td>
<td>3.90</td>
<td>0.27</td>
<td>3.91</td>
<td>0.29</td>
</tr>
<tr>
<td>7 4</td>
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<td>3.92</td>
<td>0.087</td>
<td>3.88</td>
<td>0.12</td>
</tr>
<tr>
<td>9 5</td>
<td>1.67±0.28</td>
<td>1.46</td>
<td>0.56</td>
<td>1.45</td>
<td>0.62</td>
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<tr>
<td>8 4</td>
<td>1.67±0.56</td>
<td>1.71</td>
<td>0.0051</td>
<td>1.69</td>
<td>1.28</td>
</tr>
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</table>

Table 4.4. Comparison of relative intensities for $^{32}$S$_{16}$.

Widths fed in for levels $(n,l) = (3,2)$ and $(4,3)$ for use in West's formula. Data from ref. [72].

$\alpha = 0.14$; refilling width = 0.225 eV.
<table>
<thead>
<tr>
<th>TRANSITION NO. X RAYS</th>
<th>NO. X RAYS EXPERIMENTAL</th>
<th>NO. X RAYS WEST WIDTHS</th>
<th>$\chi^2$</th>
<th>NO. X RAYS B-S WIDTHS</th>
<th>$\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n \rightarrow n$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>100.0±1.9</td>
<td>100.0</td>
<td>0</td>
<td>100.0</td>
</tr>
<tr>
<td>6</td>
<td>4</td>
<td>9.46±0.37</td>
<td>12.5</td>
<td>67.5</td>
<td>12.4</td>
</tr>
<tr>
<td>7</td>
<td>4</td>
<td>3.49±0.29</td>
<td>3.92</td>
<td>2.2</td>
<td>3.88</td>
</tr>
<tr>
<td>8</td>
<td>4</td>
<td>1.98±0.34</td>
<td>1.71</td>
<td>0.63</td>
<td>1.69</td>
</tr>
<tr>
<td>7</td>
<td>5</td>
<td>11.7±3.6</td>
<td>12.9</td>
<td>0.37</td>
<td>13.0</td>
</tr>
<tr>
<td>8</td>
<td>5</td>
<td>3.13±0.45</td>
<td>3.90</td>
<td>2.9</td>
<td>3.91</td>
</tr>
<tr>
<td>9</td>
<td>5</td>
<td>2.31±0.75</td>
<td>1.46</td>
<td>1.3</td>
<td>1.45</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>25.9±2.2</td>
<td>24.1</td>
<td>3.2</td>
<td>24.1</td>
</tr>
</tbody>
</table>

Table 4.4. Comparison of relative intensities for $^{32}$S$_{16}$.

Widths fed in for levels $(n,l) = (3,2)$ and $(4,3)$ for use in West's formula. Data from ref. [63].

$\alpha = 0.14$; refilling width = 0.225 eV.
concluded that on the whole the theoretical and experimental relative intensities agree. This is not to discount the several isolated lines which seem contrary to this conclusion. From Table 4.5, it is seen that the relative intensity, from Godfrey's data, of the $4 \rightarrow 3$ transition for $S$ is half the theoretical value. However, the Backenstoss measurement of the same line is twice as high, raising once again the possibility of error in Godfrey's experiment. Similarly, the Backenstoss value of the $9 \rightarrow 5$ relative intensity (in Table 4.6) is much higher than the theoretical value, while the Godfrey measurement is lower and more satisfactory. It would seem therefore that the conclusion above is justified.

There are no significant intensity differences from the two versions of the cascade calculations. The differences there are are negligible with respect to those existing between the two sets of experimental data. Therefore, the customary use of West's formula and the use of only a small number of widths in cascade calculations is perfectly justified. The fact that the incorrect widths which West's formula gives do not affect the calculation means that indeed the states to which those widths pertain are nearly empty.

In the cascade calculations of Godfrey, the absolute intensities tended to agree for $\Delta n = 1$ transitions but to disagree for $\Delta n = 2$. In this calculation, the absolute intensities tend to be discrepant for all values of $\Delta n$, while the relative intensities are in general harmony. This suggests that had Godfrey compared relative intensities instead, he would have secured better success. This has an implication on the current multiplicity of
forms for $P(l)$: the number of such forms could probably be reduced if only relative intensities were compared. It would appear that a difference in normalization which is not recognized sometimes spoils the agreement between theoretical and experimental absolute intensities. The effort to achieve agreement of absolute intensities in all cases is probably partly responsible for the large number of forms for $P(l)$.

Distortion of the wavefunction by the strong potential, as discussed in Chapter 2, not only prevents the use of perturbation theory to calculate the widths but affects other quantities as well. It is usual to calculate radiative and Auger rates with hydrogen-like wavefunctions (which may be corrected for the finite size of the nuclear charge, and the screening of atomic electrons from the nucleus by the kaon) but obviously, full rigour recommends the use of distorted wavefunctions. As the dipole and Auger operators have their maximum values away from the nucleus - the region of most distortion - the effect of wavefunction distortion on the respective widths is likely to be small. Nevertheless, this point is worth future attention.

As mentioned in Chapter 1, it is a frequent practice to convert the X-ray yield for the last-observed transition to a width. Theoretical knowledge of the radiative width is necessary for this, and again, there is a need to assess the correction to it due to wavefunction distortion.

In conclusion, only circular-orbit states are appreciably populated in kaonic-atom cascade, and of these only a few contribute meaningfully to the competition between radiative and absorptive depopulation of orbits, owing to the fact that the
absorptive is either negligible or overwhelming compared to the radiative width for the rest of the states. And so West's formula, despite being derived from invalid perturbation theory, is adequate for use in kaonic-atom cascade calculations.
17 Hufnner J., Hufnner cascade code CASCADE, modified by G Hunt and W. Sapp.

23 Batty C. J., "Recent Results on Kaonic and Sigma Atoms;" Paper presented at Int. Conf. on Hypernuclear and Low Energy Kaon Physics, Warsaw, 1979.
42 Batty C. J. et al, Nucl. Phys. A


71 O'Leary K., PhD Thesis, University of Surrey, 1982.


77 Keski-Rahkonen and Krause M. O., Atomic and nuclear Data Tables. 14, 139 (1974).


SECTION II

A VARIATIONAL INVESTIGATION OF THE KAONIC HYDROGEN MOLECULAR ION
The kaonic hydrogen molecular ion is studied. Due to the large value of the kaon mass in relation to the proton mass, the Born-Oppenheimer approximation and most other adiabatic methods do not apply and the variational Gaussian-expansion method is used. The ion turns out to exist only in the ground state. The binding energy of this state is given. Strong-interaction effects are found to be important, and values are given for the shift and absorption width. The kaonic-hydrogen strong-interaction shift and width for the particular potential used naturally appear. The importance of corrections which are normally small, like that due to the proton-proton nuclear force, is stressed. Some generalizations of the results to antiprotonic and sigma-hyperonic atoms are made. The Gaussian-expansion method is developed further and formulas for use in computing dipole transition matrix elements of three-body ions which possess excited states are given.
CHAPTER FIVE - THE THREE-BODY PROBLEM

SECTION 5.1 - INTRODUCTION

The number of bound three-body systems has been greatly increased by the advent of artificially-produced charged "exotic" elementary particles. Most of these systems have already come under the scrutiny of research [1-9]. A conspicuous exception is the kaonic hydrogen molecular ion. The ppK system appears to have received no attention at all, and two factors probably account for this. The first is that most current research into three-body systems is impelled by interest in muon-catalysed hydrogen fusion [1-12], while the ppK system is not of direct relevance to the topic. The second is that the mass of the kaon would seem to prohibit the use on the system of the adiabatic Born-Oppenheimer method of solution [13-16], which is usually the first avenue of attack. Yet, the kaonic hydrogen molecular ion is a system worthy of study. If there were no other reason at all, there would be the aesthetic pleasure of fitting into place one more piece in the jigsaw of knowledge. But there are more compelling motives.

Firstly, the role of the strong interaction in molecular systems is an issue of increasing interest [17]. This force is
much stronger in the ppK system than in the pionic hydrogen molecular ion and other three-body ions heretofore studied, and therefore manifests itself more strongly in this system. A feeling for its effects in the ppK case is likely to assist the understanding of $\Sigma^-$ hyperonic and anti-protonic hydrogen molecular systems. Systems involving the anti-proton and the sigma hyperon are coming more and more into the theoretical spotlight as laboratory techniques for producing heavy elementary particles improve [18,19].

Secondly, though kaonic atoms are thought to be well understood, problems remain in regard to kaonic hydrogen. For this atom, the theoretical and experimental energy shift and absorption width have not yet been satisfactorily reconciled [20-23]. In part, this problem may derive from the strong interaction itself, the form of which between a kaon and a proton has yet to be definitively given [24,25]. However, there is a possibility that unrecognised molecular effects contribute in some measure to the difficulties. It is hoped that any such effects will be detected through this work.

Thirdly, though the Born-Oppenheimer approximation would seem to be disqualified from the ppK case because of the relatively large kaon mass, it is still a matter of importance to establish how poorly it performs. For this reason, at least a rough assessment of its performance should be contrasted with that of the variational technique (which is the method to be principally used). This would serve to help define its domain of applicability, and to justify the use of an alternative method of
solution. Also there is a chance that for reasons which are perhaps hidden from present understanding, this domain is wider than might be expected. Many a theory in Physics has confounded a priori analysis by yielding reliable results under conditions for which it was not originally devised.

Lastly, this work should function as a guide to experiments on the ppK ion.

The specific aims in this section of the thesis are to calculate basic quantitites for the ppK ion; these are

(a) the energies of the bound states,

(b) the energy shift due to the strong interaction between the meson and the protons,

(c) the rate of nuclear absorption of the kaon resulting from the strong interaction,

and

(d) the expectation values of various powers of inter-particle distances.

In addition, formulas with which to calculate dipole-transition radiative probabilities are given in one of the appendices, so that an estimate to X-ray intensities can be made.

SECTION 5.2 - PLAN OF SECTION II OF THE THESIS

This chapter of the thesis is devoted to a sketch of the two main approaches to solving the three-body system, with particular emphasis on the adiabatic method and its shortcomings. The more appropriate variational method is briefly touched upon, but is
considered in greater theoretical detail in Chapter 6. Chapter 7 contains the specialization of the variational technique to this special problem. A discussion of calculational details in Chapter 8 precedes the presentation of the results. Finally, these are discussed and commented upon in the Chapter 9, which also contains the conclusion. Appendix A contains the transformation of the three-body Hamiltonian from laboratory coordinates to internal coordinates. Appendix B contains the explicit derivation of one of the matrix elements given in Chapter 7. Appendix C is devoted to the derivation of the radiative dipole matrix element, and Appendix D contains the expression for the probability density.

SECTION 5.3 - THE THREE-BODY SCHROEDINGER EQUATION

The fundamental problem facing the application of quantum mechanics to systems containing more than two particles is that no matter what frame of reference is used, the various coordinates are too intimately mixed for the partial differential equation to separate into a number of ordinary differential equations. Over the years, two main classes of methods have evolved in the effort to overcome this problem: the adiabatic and the variational. The basic logic of the adiabatic method restricts its simpler and cruder versions to systems in which there is a mass asymmetry, though sophisticated versions manage to apply more comprehensively. The variational method is perfectly valid in all systems and is for this reason favoured in this thesis. However,
in molecular quantum mechanics, the adiabatic Born-Oppenheimer approximation is probably the best-established of all three-body approximation methods, and it is necessary to clearly show why another method is preferred. This task requires the initial steps in the formulation of the three-body problem, and they are now given in detail because they are preliminary to a variational treatment as well.

In the laboratory system of coordinates, the particles are identified by the masses \( m_1 \), \( m_2 \) and \( m_3 \), with respective displacements \( x_1 \), \( x_2 \) and \( x_3 \). The Hamiltonian operator is

\[
H = -\frac{\hbar^2 V_1^2}{(2m_1)} -\frac{\hbar^2 V_2^2}{(2m_2)} -\frac{\hbar^2 V_3^2}{(2m_3)} + V(x_1, x_2, x_3). \tag{5.1}
\]

Usually the potential \( V \) is a function of inter-particle distances and mixes the nine laboratory coordinates, so that the problem is not easily solved in this coordinate system. Actually, at least three of the coordinates are superfluous, since they describe the motion of the centre of mass. In the absence of external influences on the system, this motion is constant and is of no interest. The three-body system shares this property with all other many-body systems, since quite generally, the Hamiltonian always commutes with translations of the centre of mass [26]. This fact can be exploited by transforming to a system of coordinates in which the terms either contain the centre-of-mass coordinates alone or they do not at all. It is possible to do this if the potential energy is a function of
interparticle distances alone. Formally, this is accomplished by the general transformation of coordinates [27-33]

\[ X = \frac{(m_1x_1 + m_2x_2 + m_3x_3)}{M}, \quad (5.2) \]
\[ r = x_2 - x_1, \quad (5.3) \]
\[ R = x_3 - \frac{(\beta_1x_1 + \beta_2x_2)}{(\beta_1 + \beta_2)}, \quad (5.4) \]

where

\[ M = m_1 + m_2 + m_3. \quad (5.5) \]

It results in the Hamiltonian changing to

\[
H_t = -\hbar^2 \nabla_X^2 / (2M) - \frac{\hbar^2}{2M_a} \left[ \nabla_r^2 + \frac{a}{2}(\nabla_r \nabla_r^2) \right] - \frac{\hbar^2}{2M_a} \nabla_R^2 - \frac{\hbar^2}{2M_a} \nabla_R^2 \left[ \nabla_R \nabla_R \right] - \frac{\hbar^2}{2M_a} \nabla_R^2 \quad (5.6)
\]

where

\[ a = \frac{(m_2 - m_1)}{(m_2 + m_1)} - \frac{(\beta_2 - \beta_1)}{(\beta_2 + \beta_1)}, \quad (5.7) \]

with \( \beta_1 \) and \( \beta_2 \) chosen according to the type of approximation to be made. The masses are

\[ M_a^{-1} = m_1^{-1} + m_2^{-1}, \quad (5.8) \]

and
\[
m_a^{-1} = m_3^{-1} + (m_1 + m_2)^{-1}.
\] (5.9)

In the formulas above, the choice of \( r \), and dependently that for \( R \), is arbitrary, since the difference of any two laboratory-system displacements is equivalent to the one chosen. Altogether, there are three sets of equivalent transformations. A more complete discussion of these transformations is undertaken in Chapter 7. The transformation of the Hamiltonian which accompanies each such choice is fully derived in Appendix A.

Only the first term on the right-hand side of (5.6) is a function of \( X \). A product form for the wavefunction

\[
\phi(X,r,R) = \chi(X)\psi(r,R)
\] (5.10)

results in the Schroedinger equation separating into two parts

\[
-\hbar^2 \nabla_X^2 \chi(X) = 2ME_{cm}^\chi(X)
\] (5.11)

and

\[
H\psi(r,R) = E\psi(r,R),
\] (5.12)

where

\[
H = -(h^2/2M_a)[\nabla_r^2 + (a/2)(\nabla_R \nabla_r + \nabla_r \nabla_R) + (a^2/4)\nabla_R^2] - \hbar^2/2m_a) + V(r,R).
\] (5.13)
In (5.12), $E_{cm}$ is the energy of the motion of the centre of mass and $E$ is the internal energy of the system.

Insofar as the number of coordinates has been reduced to six from the original nine, (5.13) represents a considerable simplification of the system. Nevertheless, the Schroedinger equation is still intractable; it is at this point that approximations are made. The first class of approximation is the adiabatic method.

SECTION 5.4 - THE ADIABATIC APPROXIMATION

In the adiabatic method, the wavefunction is expanded in terms of the so-called adiabatic basis. These are the wavefunctions for a negatively-charged particle moving in the Coulomb field of two positively-charged particles at rest. For the particular coordinates defined in the last section, the clamped particles would take the labels 1 and 2. In terms of the adiabatic basis, the solutions are [14]

$$\psi (r,R) = \sum \varphi_1 (r,R) \psi_1 (r), \quad (5.14)$$

where the $\varphi_1$ are the solutions of the two-centre problem and the $\psi_1$ are expansion coefficients.

The two-centre problem is separable in confocal elliptical coordinates [34], for which $\beta_1 = \beta_2 = 1$; this choice corresponds to measuring the displacement of the third particle from the geometrical centre of the line joining particles 1 and 2. If in
addition \( m_1 = m_2 \), the internal Hamiltonian (5.13) becomes [27-33]

\[
H = -(\hbar^2/2M_a)\nabla^2_r - (\hbar^2/2m_a)\nabla^2_R + V(r,R), \tag{5.15}
\]

and the two-centre problem is

\[
-(\hbar^2/2m_a)\nabla^2_R \varphi_1(r,R) + V(r,R)\varphi_1(r,R) = \epsilon_i \varphi_1(r,R), \tag{5.16}
\]

where \( \epsilon_i \) is the energy for the two-centre solution characterised by the quantum number \( i \).

Since particles 1 and 2 are fixed for the purpose of computing the two-centre wavefunctions, \( \varphi(r,R) \) is really a parametric function of \( r = |r| \), which appears only in the term for the Coulomb interaction between the fixed positive charges. The term is a constant which has the effect of altering the origin of energy measurement; it can therefore be ignored and added to the two-centre energy after solution. Thus the two-centre problem changes from

\[
-(\hbar^2/2m_a)\nabla^2_R \varphi_i - (e^2/r_{13} + e^2/r_{23} - e^2/r)\varphi_i = \epsilon_i \varphi_i \tag{5.17}
\]

to

\[
-(\hbar^2/2m_a)\nabla^2_R \varphi_i - (e^2/r_{13} + e^2/r_{23})\varphi_i = \epsilon_i \varphi_i \tag{5.18}
\]

where \( r_{kl} \) is the separation of particles \( k \) and \( l \). The connection between \( \epsilon_i \) and \( \epsilon_i \) is
Obviously, the choice of \( r \) is such that \( r = r_12 \).

The solutions of (5.17) are ultimately obtained numerically. Tabulations have been made and are available in the literature [31,35-38]. The two-centre problem is a field of study in its own right; an example of the literature devoted to it is provided by references [39-55].

On inserting the series (5.14) into (5.12), multiplying by \( \phi_j^* \) and integrating over the coordinates of the two-centre problem, an infinite system of integro-differential equations is obtained for the coefficient functions \( \psi_i \) [31,38,56]. Thus (5.12) becomes

\[
-(h^2/2M_a) \sum \int_{ \sigma_{1,1} } \phi_j^* \partial^2 \phi_{1,1} r \psi_i dR + \sum \int \phi_j^* H_o \phi_1 dR \psi_i = \sum \int \phi_j^* \phi_1 dR \psi_i,
\]

where \( H_o \) is the Hamiltonian of the two-centre problem given by expression (5.16).

Using the orthogonality of the members of the adiabatic basis, and the well-known vector identity

\[
\nabla^2 (f_1 f_2) = f_1 \nabla^2 f_2 + f_2 \nabla^2 f_1 + 2 \nabla f_1 \cdot \nabla f_2,
\]

where \( f_1 \) and \( f_2 \) are appropriate functions, (5.19) is recast as

\[
-(h^2/2M_a) \nabla^2 \psi_j + (\epsilon_j + e^2/r - E) \psi_j,
\]

\( \varepsilon_i = \varepsilon_1 - e^2/r. \)
\[ = \left( \frac{\hbar^2}{2M_a} \right) \Sigma_i \left[ \mathbf{\nabla}_i \psi_i \cdot \mathbf{\nabla} \psi_i + \psi_i \mathbf{\nabla}^2 \psi_i \right] \] (5.20)

for every j.

Various degrees of the adiabatic approximation are distinguished by the extent to which terms on the right-hand side of (5.20) are ignored to facilitate solution [57,58]. The most drastic form is the Born-Oppenheimer approximation [13-16], in which the right-hand side is discarded altogether.

SECTION 5.5 - THE BORN-OPPENHEIMER APPROXIMATION

The Born-Oppenheimer approximation is designed for cases where one of the three masses is much smaller than the other two. Then, the larger masses move much more slowly than the smaller one, and in the periodic time of the motion of the latter, the former have hardly shifted position at all. Thus, the energy of the motion of the light particle is accurately given by the solutions of the two-centre problem. When this has been completely solved, the functional dependence of \( \varepsilon \) on \( r \) is obtained. Together with the electrostatic interaction between the two heavy particles, this energy is effectively a potential governing the motion of these two particles. The Schroedinger equation to be solved for this motion is precisely (5.20) with the right-hand side left out.

The smaller the ratio of the smaller mass to the reduced mass of the two larger ones, the better the Born-Oppenheimer approximation. For this reason, the hydrogen molecular ion is particularly well-approximated in this picture, and was studied by
this means early on [15,16]. Mesonic systems are more crudely depicted, since the negative particle is at least 200 times larger, but even here, for excited states, the approximation has achieved fair results [59].

For the ppK system, the ratio of the kaon to the reduced mass of the two protons is almost unity. It therefore appears unlikely that the Born-Oppenheimer method can be profitably applied to this ion. To see this more clearly, it is useful to view the Born-Oppenheimer method from another perspective. If the total potential energy and the kinetic operator for the light particle are taken as constituting the initial Hamiltonian, the three-body problem can be solved by perturbation theory with the kinetic operator of the other two particles as the perturbation [13,60]. This procedure is equivalent to the approach that has been taken so far. The zeroth-order solutions for the wavefunction and the energy are the two-centre wavefunctions. The complete series solutions are in terms of the expansion parameter

$$\kappa = (m_k/\mu)^{1/4},$$

where $m_k$ is the kaon mass and $\mu$ the proton-proton reduced mass. The Born-Oppenheimer approximation results from taking the first two terms only in each series. It is evident that since the expansion parameter is almost unity for the ppK case, this constitutes a serious over-simplification of the actual solution. The convergence of the perturbation series is in doubt and the first few terms may constitute no great fraction of either the
energy or the probability density.

Even if the Born-Oppenheimer approximation was valid in the ppK case, considerable difficulty would have to be surmounted to deal with the strong interaction. The strong-interaction terms in the Hamiltonian would be associated with the two-centre problem, which would necessitate anew the labour of solving it. Perturbation theory might be considered as an alternative, but as has been discussed in Section 1, Chapter 2, its use in kaonic systems is not straightforward. The complex energy shift is small enough relative to the total energy to satisfy the first condition for the validity of this procedure. But this on its own is not sufficient; in addition, the perturbation must not result in the new system having a greatly-changed wavefunction from the original. Unfortunately, the wavefunction does get badly distorted in the vicinity of kaonic-system nuclei (as discussed more fully in Chapter 2).

SECTION 5.6 - AN ESTIMATE OF THE VALIDITY OF THE BORN-OPPENHEIMER APPROXIMATION IN A GIVEN CASE

According to the Born-Oppenheimer approximation, the energy of the three-body system is comprised of several parts. The first contributions $\epsilon_j$ is due to the motion of the light negatively-charged particle in the Coulomb field of the two heavy particles. The second contribution $E_{vib}$ comes from vibrations of the heavy nuclei about their positions - for, although the two-centre problem was solved for a series of inter-particle
distances, the two nuclei are actually in the vicinity of the equilibrium separation $r_0$ which is simply given by the separation at which the potential energy is minimum. This potential is

$$u(e_j, r) = e_j + e^2/r.$$ (5.21)

There is a third contribution to the energy, due to rotation of the ion, but it is much smaller than the first two contributions.

In the picture just sketched, the condition for validity of the Born-Oppenheimer method is that the vibrational energy should be much smaller than the energy of the light particle. The ratio of the two energies can always be found after the calculation has been performed; however, a simple estimate based on the Uncertainty Principle gives a good answer to the question [61].

If the linear dimensions of the molecular ion are of order $d$, then the negative particle has an energy, by the Uncertainty Principle,

$$\varepsilon = \hbar^2/(m_3 d^2),$$ (5.22)

from which is deduced an expression for the energy by replacing $d$ by the inter-nuclear distance $r$. $m_3$ is the mass of the light particle.

The energy of vibration of the nuclei is

$$E_{vib} = \hbar(k/\mu)^{1/2},$$ (5.23)
where $\mu$ is their reduced mass and $k$ is a harmonic-oscillator force constant.

Since the heavy particles stay in the vicinity of the equilibrium separation, it is a good approximation to express the potential energy near that point in a power series in the parameter $(r-d)$. The linear term necessarily vanishes and the first two terms in the expansion only are retained. The contribution to the derivative from the second term in (5.21) vanishes because the two nuclei stay in the vicinity of the equilibrium position and their electrostatic repulsion is constant. Thus,

$$u = -D + k(r-d)^2/2, \quad (5.24)$$

where $D$ is the dissociation energy. Comparing the expression to the Taylor expansion, the value of $k$ is found as

$$k = \left(\frac{\partial^2 \varepsilon}{\partial r^2}\right)_{r=d}, \quad (5.25)$$

and from (5.22),

$$k = \varepsilon/d^2. \quad (5.26)$$

Thus,

$$E_{\text{vib}} = \hbar\varepsilon/\mu d^2 \approx \hbar^2/2(m\mu)^{1/2} \approx \varepsilon(m\mu)^{1/2}, \quad (5.27)$$
so that finally,

\[ E_{\text{vib}}/e \approx (m_2/\mu)^{1/2}. \] 

(5.28)

As an order-of-magnitude estimate, this formula is fairly good. For the ordinary hydrogen molecular ion, it predicts a ratio of 3.2% (as opposed to the actual value of 2% [62]). For the pionic hydrogen molecular ion, it gives 54%, while the exact value is 34% [59]. The high ratio for the latter case indicates that the application of the Born-Oppenheimer method to that ion is doubtful; indeed the ground-state energy of -243.1 eV obtained in [59] compares unfavourably with the more reliable value of -294.7 eV found here in an application of the variational method.

On using the formula on the ppK system a ratio of 1.03 is found. This ratio confirms what fundamental considerations had suggested: the Born-Oppenheimer technique cannot be used reliably on the ppK ion.

SECTION 5.7 - FURTHER COMMENTS ON THE ADIABATIC METHOD

Higher-order terms in the perturbation series arise from the "adiabatic corrections" on the right-hand side of (5.20). Much effort has gone into the computation of at least some of these terms [10,31,38,63-72]. But because of the size of the expansion parameter in the ppK case, these corrections probably exercise little or no influence on the accuracy.
It is necessary to modify the pure adiabatic method in order to widen its scope to comprehend such systems as the ppK ion. The task has been addressed \[31,38,56\] and consists in admixing some variational aspects into the formulation. Though the design is achieved, it is at the price of excessive complexity. In contradistinction, the pure variational method is much more straightforward to use, and for this reason is preferred here.

An extensive literature attests to the success of the adiabatic method on appropriate systems. The papers listed in this chapter together with references \[73-81\] lead by cross-reference to the bulk of the remainder of the literature.

SECTION 5.8 - THE VARIATIONAL METHOD

The variational method is applied to a system by guessing a form for the wavefunction and using it to compute the expectation value of the energy. The procedure is based on the fact that for the ground state of the system in every case, and for the excited states if the trial functions are selected in a certain way, the approximation to the energy has certain bounding properties in relation to the actual value \[82\]. These bounds facilitate a systematic method of improving the test functions, and thereby the approximations to the energies. Good choices of the trial functions, possible by careful analysis of the Hamiltonian, lead to very accurate energies and wavefunctions.

The variational technique is perfectly general inasmuch as it is not constrained by the values which the particle masses may
assume. However, as in many other problems, the coordinates in which the problem is expressed are an important issue. They partly dictate the choice of trial function, and in conjunction with one another, these two factors are responsible for a diversity of formulations in the literature. Of the numerous variants, the Gaussian-expansion method of Kamimura [17,83-85] is used in this thesis.

The possibilities of the variational technique have been exploited in molecular quantum mechanics from the very earliest days. As early as 1929, the ground state of the helium atom had been studied by that means [86]. Numerous other applications on a wide range of systems have followed that example over the years. A sample of the literature is given by references [2-5,87-93]. A noticeable feature of these calculations, is that they are confined to the ground state. For excited states, variational calculations tend to suffer from excessive complexity, unless the trial function is chosen very restrictedly.

The theorems underlying the variational method are presented with some rigour in the next chapter. Detailed discussion is deferred to that occasion.
CHAPTER SIX - THE THEORY OF THE VARIATIONAL METHOD

SECTION 6.1 - THE FOUNDATIONS OF THE VARIATIONAL METHOD

In this chapter, a systematic basis for the use of the variational method in obtaining approximate wavefunctions and energies for a quantum-mechanical system is established. The variational technique pervades the solution of problems in Physics and Mathematics and for this reason expositions of it are common in books on differential equations; an example is the text by Kopal [94]. Originally, the method was developed by Rayleigh [95], Weber [96], Poincare' [97], Fischer [98], Polya [99] and Weyl [100,101]. The material contained in this chapter is composed from the texts by Epstein [82], Weinsten and Stenger [102], Gould [103], and Kopal.

In quantum mechanics, the variational method is built around the expectation value of the energy of the system under consideration. For any trial function \( \psi \), the expectation value of the energy is

\[ E = \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle, \]  

(6.1)

where \( H \) is the Hamiltonian operator for the system. The following
Theorems relating to $E$ and $\psi$ constitute the foundations of the variational approximation.

Theorem 1: If the trial function $\psi$ is thought of as being a continuously variable quantity, the eigenvalues of $H$ are stationary points of $E$ as a functional of $\psi$.

Theorem 2: $E$ in (6.1) has no stationary points apart from those which correspond to eigenvalues of $H$, and a trial function which corresponds to a stationary point is an eigenfunction of $H$.

Theorem 3: The smallest eigenvalue of $H$ is not only a stationary point of $E$ as a functional of $\psi$ but is the absolute minimum. The higher eigenvalues are saddle points.

Theorem 4: The states of $H$ may be classed into types according to any constraining principle on the system or other observables which commute with the Hamiltonian, and the smallest eigenvalue of $H$ for states of a given type is the absolute minimum of $E$ as a functional of that type of trial functions.

Theorem 5: Theorems 1 and 2 apply separately to the eigenfunctions and eigenvalues of each distinct type.

Theorem 6: If the trial function in (6.1) is chosen to be orthogonal to eigenfunctions associated with eigenvalues smaller
than a given value of $E$, then this eigenvalue is an absolute minimum with respect to trial functions of the new type.

SECTION 6.2 - COMMENTS ON THE THEOREMS

Theorems 1-6 almost suffice to sustain the variational method in practical calculations. According to Theorem 1, the methods of calculus for locating the stationary points of a function of several variables can be directly adopted to find the eigenvalues of $H$ once a good choice for the trial wavefunction has been made. A little reflection shows that the value of this theorem is weakened or perhaps destroyed if some of the stationary points of $E$ in (6.1) do not correspond to eigenvalues. It is an important question whether any of the stationary points are spurious from the quantum-mechanical viewpoint, and need to be sifted from those which are actually approximations to the energy. It is this very problem which Theorem 2 addresses and resolves. Every stationary point of $E$ as a functional of $\psi$ is an approximation to an eigenvalue.

The next question of interest is the accuracy of the approximate eigenvalues. For the lowest eigenvalue of a Hamiltonian, the answer is supplied by Theorem 3. The variational method always over-estimates the energy. An improvement in the trial function is manifested in a lower approximation to this eigenvalue.

Unless the excited state is of a different symmetry or type from the state of lowest energy, Theorems 1-6 do not make any
statement about approximations to its energy. This question has not been resolved in general, and a partial answer to it awaits a particular specialization of the variational method - the so-called linear-variation method. However, if this state is indeed distinct in symmetry or type from other states of the Hamiltonian, then the approximation to its energy is always too high, because Theorem 4, which is evidently a generalisation of Theorem 3, applies to it. As a matter of fact, the value of Theorem 4 goes beyond this; this theorem makes possible the application of the variational method in practice. The lowest energy of the Hamiltonian does not necessarily define the ground state of a system. For example, though the 1s state in an atom is the ground state, the Pauli exclusion principle prevents all but two electrons from occupying it. If Theorem 3 applied only to the absolute lowest state of the system, the variational calculation would yield the erroneous result that all the electrons in an atom occupied the 1s state. It is therefore an important result that to get physical ground-state energies, all that need be done is to incorporate the principle which differentiates the various states of the system into the test function.

According to Theorem 5, Theorem 2 applies to eigenvalues and eigenfunctions of states of any type. Therefore, the principle that every stationary point is an approximation to some eigenvalue embraces every class of states.

Theorem 6 is a generalization of Theorem 4 for the purpose of finding the next higher eigenvalue once all the smaller ones have been located. If the new trial function has been chosen so
as to be orthogonal to those for the energies already found, then it obviously belongs to a different type and must correspond to one of the higher eigenvalues. If all such trial functions are used in (6.1), then the required next state is defined by the smallest energy found. In this way, in theory at least, all the solutions for a given Hamiltonian can be systematically constructed.

SECTION 6.3 - PROOFS OF THE THEOREMS

Proof of Theorem 1.

In (6.1) let ψ' be another trial function differing from ψ by a quantity Δ. Thus

\[ \psi = \psi' + \Delta, \] (6.2)

so that while

\[ E = \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle, \] (6.1)
\[ E' = \langle \psi' | H | \psi' \rangle / \langle \psi' | \psi' \rangle. \] (6.3)

Inserting (6.2) in (6.1) yields

\[ E = (E'\langle \psi' | \psi' \rangle + \langle \psi' | H | \Delta \rangle + \langle \Delta | H | \psi' \rangle + \langle \Delta | H | \Delta \rangle) / \langle \psi | \psi \rangle. \] (6.4)

From (6.2) it follows that
\[ E' \langle \psi' | \psi' \rangle = E' (\langle \psi | \psi' | - \langle \psi' | \Delta > \langle \Delta | \psi' > - \langle \Delta | \Delta > ) , \] 

(6.5)

so that after inserting (6.5) in place of the first term on the right-hand side of (6.4), the expression

\[ E = E' + \frac{\langle \psi' | (H-E') | \Delta > + \langle \Delta | (H-E') | \psi' > + \Delta | (H-E') | \Delta >}{\langle \psi | \psi >} \] 

(6.6)

is obtained. Since \( H-E \) is Hermitian,

\[ \langle \psi' | (H-E') | \Delta > = <(H-E)|\psi' | \Delta > , \] 

(6.7)

and so (6.6) becomes

\[ E = E' + \frac{\langle (H-E') \psi' | \Delta > + \langle \Delta | (H-E') | \psi' > + \langle \Delta | (H-E') | \Delta >}{\langle \psi | \psi >} \] 

(6.8)

If \( \psi' \) is an actual eigenfunction of \( H \), then by definition,

\[ (H-E') \psi' = 0 . \] 

(6.9)

In that case, the energy given by the approximation \( \psi \) is

\[ E = E' + \langle \Delta | (H-E') | \Delta > / \langle \psi | \psi > \]. \] 

(6.10)

Thus, the difference between the exact energy \( E' \) and the approximation \( E \) is second-order in the difference between the wavefunctions. The vanishing of the first-order terms in \( \Delta \) is
precisely the condition that defines the stationary points of $E$ as a functional of $\psi$. Thus Theorem 1 is proved.

Proof Of Theorem 2.

Let $E'$ be a stationary point of $E$. This means that the first-order terms in (6.8) vanish for every choice of $\Delta$. Thus

$$<(H-E')\psi'|\Delta> + \Delta<(H-E')\psi'> = 0,$$

(6.11)

for every choice of $\Delta$. If it is possible for $E'$ to be a stationary point of $E$ but not an eigenvalue of $H$, then $\Delta$ can be chosen as

$$\Delta = \alpha(H-E')\psi',$$

(6.12)

where $\alpha$ is a continuously variable number. Using (6.12) in (6.11), the equation

$$(\alpha^* + \alpha)<(H-E')\psi'|(H-E')\psi'> = 0,$$

(6.13)

is obtained. Therefore, unless $\alpha = 0$,

$$(H-E')\psi' = 0,$$

(6.14)

and Theorem 2 is verified.
Proof Of Theorem 3.

This readily proceeds from (6.10). If $E'$ is the ground-state energy, then $(H-E')\psi$ is always positive, and since $\Delta$ can be thought of as a linear combination of $\psi$'s, it follows that $\langle \Delta | (H-E') | \Delta \rangle$ is positive as well. Hence the approximation $E$ is always greater than the actual eigenvalue $E'$ unless by fortuitous choice $\psi$ is the actual eigenvalue — in which case $E$ and $E'$ are equal. For the higher eigenvalues for that class of solution, different choices of $\Delta$ make the correction either positive or negative, since for each eigenvalue, there is at least one lower one. Hence, indeed, these eigenvalues are saddle points of $E$ as a functional of $\psi$.

Proof Of Theorem 4.

The choice of trial function must be patterned after the form of the actual solution. The actual eigenfunctions are orthogonal to each other if they belong to different values of a conserved quantity which commutes with the Hamiltonian or if they belong to different symmetries. The conserved quantities or the symmetries are known beforehand, and are reflected in the construction of the test functions. As a result, the trial functions for different classes of solution are orthogonal to one another. For each class of solution, the variation $\Delta$ is of the same type and so can be thought of as a linear combination of trial functions of that type. Hence the different types of $\Delta$ are
orthogonal to one another, and the argument of Theorem 3 applies to each class of solution independently of all others.

Proof of Theorem 5.

The proof follows the same reasoning as that of Theorem 4. In Theorem 2, the arbitrary variation $\Delta$ is necessarily of the type or symmetry of the state under consideration, which means that this theorem applies separately to each class of solution.

Proof of Theorem 6.

The proof of this theorem proceeds from Theorem 4. If Theorem 4 is applied systematically to find the lowest eigenvalue of each class of solution - moving up in energy from one class to the next - then at each stage by definition, only trial functions of a type distinct in the orthogonality sense from the eigenfunctions for lower eigenvalues than $E'$ are allowed. Since $\Delta$ is now a linear combination of functions whose eigenvalues are higher than or at best equal to $E'$, it follows that

$$\langle \Delta | (H-E) | \Delta \rangle \geq 0.$$  

With the theorems proved, the question of implementing them is addressed. For the lowest energy of each class of solution, it is immediately obvious how to do this. Trial functions which conform to the constraints on the system are chosen with
parameters which can be varied to lower the energy as much as possible. The best trial function is the one yielding the lowest energy, and the job is done when this energy is constant to the desired number of decimal digits. So far as the excited states are concerned, no procedure is yet deducible, since the bounding relationships, if any, between the actual and approximate eigenvalues are unknown. These rules could probably be derived case by case [104,105], but there is one situation in which they are generally known - the case when the parameters to be varied occur linearly in the trial function [106-109]. This is the linear-variation method, also popularly known as the Rayleigh-Ritz method [95].

SECTION 6.4 - THE LINEAR-VARIATION METHOD

Generally speaking, the restrictions on the form of functions admissible as trial functions in the variational method, are dictated by the boundary conditions, the symmetry of the system and the set of observables commuting with the Hamiltonian. A practical constraint arises from the necessity to find the stationary points of the expression (6.1) for E. The most obvious search method is differentiating (6.1) with respect to the variational parameters and equating the first derivates to zero to obtain the values of the parameters at the critical points. Of all trial functions, the most amenable to such a procedure is the series
\[ \psi = \sum_{i=1}^{N} c_i \phi_i , \]  

(6.15)

where the only parameters to be fixed by differentiating are the linearly-occurring coefficients \( c_i \). Other parameters may be incorporated non-linearly in the \( \phi_i \), but these are fixed otherwise. Their purpose is to improve the suitability of the basis functions \( \phi_i \) to the system at hand and thereby to limit the number of terms in the series.

When (6.15) is used in (6.1), the expression to be examined for stationary points becomes

\[ E = \sum_{i,j=1}^{N,N} c_i^* c_j^* \langle \phi_i | H | \phi_j \rangle / \sum_{i,j=1}^{N,N} c_i c_j \phi_i^* \phi_j \]  

(6.16)

Neither orthogonality nor normalisation of the \( \phi_i \) has been assumed, although both are computational advantages.

The first derivative of \( E \) with respect to each of the \( c_i \) vanishes at the critical points:

\[ \frac{\partial E}{\partial c_k} = \frac{\Sigma_i c_i^* \phi_i^* | H | \phi_k \rangle}{\Sigma_i \Sigma_j c_i^* c_j^* \phi_i^* \phi_j} - \frac{\Sigma_i \Sigma_j c_i^* c_j^* \phi_i^* | H | \phi_j \rangle \Sigma_i c_i^* \phi_i | \phi_k \rangle}{\left[ \Sigma_i \Sigma_j c_i^* c_j^* \phi_i^* \phi_j \right]^2} \]

\[ = \frac{\Sigma_i c_i^* \phi_i^* | H | \phi_k \rangle - E \phi_k | \phi_k \rangle}{\Sigma_i \Sigma_j c_i^* c_j^* \phi_i^* \phi_j} = 0, \]  

(6.17)

for \( k = 1,2,\ldots,N \). \( E \) is given by (6.16).

Since the norm of \( \psi \) is necessarily non-vanishing, the system
of equations to be solved for the $c^*_i$ at the stationary points is

$$\Sigma_i c_i (\langle \phi_i | H | \phi_k \rangle - E \langle \phi_i | \phi_k \rangle) = 0,$$

(6.18)

for $k = 1, 2, \ldots, N$.

The complex conjugate of (6.18) is equivalent:

$$\Sigma_i (\langle \phi_k | H | \phi_i \rangle - E \langle \phi_k | \phi_i \rangle) c_i = 0,$$

(6.19)

for $k = 1, 2, \ldots, N$.

Equation (6.19) is a linear system of $N$ homogeneous equations. A familiar argument supplies the eigenvalues $E$. For the solutions for the $c_i$ to be non-trivial, the determinant

$$D = \begin{vmatrix} H_{11} - E_1 & H_{12} - E_1 & & H_{1N} - E_1 \\ H_{12} - E_1 & H_{22} - E_2 & & \vdots \\ & & \ddots & \vdots \\ H_{1N} - E_1 & \cdots & & H_{NN} - E_N \end{vmatrix}$$

(6.20)

must vanish. In the determinant, the matrix elements are

$$H_{i,j} = \langle \phi_i | H | \phi_j \rangle,$$

(6.21)

and

$$O_{i,j} = \langle \phi_i | \phi_j \rangle.$$

(6.22)

The equation $D = 0$ defines a polynomial of degree $N$ in $E$ and
therefore gives $N$ eigenvalues for the type of state defined by the trial function.

The main problem has reduced to the solution of the generalised matrix eigenvalue equation $Ax = \lambda Bx$, where the elements of $A$ are given by (6.21) and the elements of $B$ by (6.22). There are as many sets $x$ of variational coefficients as there are basis functions, and each set defines an approximation to one of the first $N$ eigenfunctions of the system. Generally, the accuracy of both approximate energy and wavefunction decreases rapidly with increased eigenvalue.

Since the linear-variation trial function is an expansion in terms of a basis set, the representation of the actual wavefunction by the approximation is exact if there is an infinite number of terms in the expansion. It is therefore to be expected that increasing the number of terms leads to an improvement in the energies and eigenfunctions. This is indeed the case, and is shortly to be proved. It is also to be shown that similarly to the case of the lowest energy, the linear-variation trial function leads to estimates which are too high for the energies of the excited states.

SECTION 6.5 - PROPERTIES OF THE SPACE SPANNED BY THE BASIS FUNCTIONS

The basis functions in a linear-variation trial function of $N$ terms form an $N$-dimensional linear space, provided they are linearly independent. It will now be shown that within this
space, the approximate eigenfunctions and eigenvalues of $H$ are
exact eigenfunctions and eigenvalues of another Hamiltonian $\mathcal{H}$.

Let $\Pi$ be a Hermitian projection operator which from the
universe of all functions $H$ acts upon picks out those in the
linear space.

\[
\Pi \phi = \phi, \text{ if } \phi \text{ is in the space,} \quad (6.23a)
\]
\[
\Pi \phi = 0 \text{ if } \phi \text{ is not in the space.} \quad (6.23b)
\]

Correspondingly, there is a "projected" Hamiltonian given by

\[
\mathcal{H} = \Pi H \Pi, \quad (6.24)
\]

associated with them. Any function not in the linear space can be
thought of as an eigenfunction of $\mathcal{H}$ with zero eigenvalue, as is
shown by using the second equation in (6.23):

\[
\mathcal{H} \phi = \Pi H \Pi \phi = 0. \quad (6.25)
\]

As the eigenfunctions for the non-zero eigenvalues of $\mathcal{H}$ are
orthogonal to these, it follows from Theorem 6 that the
non-vanishing eigenvalues are obtained by using trial functions in
the linear space. (One of the eigenfunctions of $\mathcal{H}$ may have zero
eigenvalue of course, but a distinction is to be retained between
that sort of vanishing of the eigenvalue and that pertaining to
the eigenvalues for states which cannot be described by the basis
set). Hence if $\psi$ is a linear combination of the basis functions,
the stationary points of $\langle \psi | h | \psi \rangle / \langle \psi | \psi \rangle$ yield approximations to the eigenvalues of $h$. However, from (6.23) and (6.24) above, it is observed that

$$
\frac{\langle \psi | h | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\langle \psi | \pi H \pi | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\langle \pi \psi | H | \pi \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \langle \psi | H | \psi \rangle
$$

(6.26)

Thus the exact eigenvalues and eigenfunctions of $h$ are approximate eigenvalues and eigenfunctions of $H$. This important result makes the proofs of various properties of the linear-variation method easier.

Since $h$ has all the formal properties of a Hamiltonian, the relations

$$
\langle \psi_k | \psi_1 \rangle = \delta_{k1},
$$

(6.27)

and

$$
\langle \psi_k | h | \psi_1 \rangle = \hat{E}_1 \delta_{k1}
$$

(6.28)

hold. Normalization has been assumed without loss of generality. $\hat{E}_k$ is an exact eigenvalue of $h$ and $\hat{\psi}_k$ is the corresponding exact eigenfunction. The $\hat{\psi}_k$ represent a re-arrangement of the basis functions to obtain a new basis set defined in terms of the $N$ mutually-orthogonal trial functions which are possible from them.
The first result to be proved using the projected Hamiltonian and its solutions is

\[ E_k \geq E'_k, \text{ for } k = 1, 2, \ldots, N , \] (6.29)

which is evidently a generalisation of Theorems 3 and 4, since it states that \( \hat{E}_k \), the \( k \)-th eigenvalue of \( \mathcal{H} \), is always a higher bound to the actual value \( E'_k \). To reiterate: since \( \hat{E}_k \) equals an approximate eigenvalue from the trial function \( \psi \), eq. (6.29) states that all excited energies from the linear-variation method are, like the lowest energy for a given class of states, always higher than the exact values. The proof is as follows.

The \( N \) eigenfunctions of \( \mathcal{H} \) form a linear space \( \{ \psi_i \} \) in terms of whose members a function \( \psi \) can be expressed thus:

\[ \psi = \sum_i \alpha_i \psi_i . \] (6.30)

The energy in the state \( \psi \) is

\[ E = \frac{\langle \psi | \mathcal{H} | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\langle \psi | \mathcal{H} | \psi \rangle}{\langle \psi | \psi \rangle} \]

\[ = \frac{\sum_{i,j} \alpha_i^* \alpha_j <\psi_i|\psi_j>}{\sum_i \sum_j \alpha_i^* \alpha_j <\psi_i|\psi_j>} = \frac{\sum_j |\alpha_j|^2 \hat{E_j}}{\sum_j |\alpha_j|^2} . \] (6.31)

\( E \) in (6.31) is an average, and so cannot be greater than the
biggest energy $E_1$ for which $\alpha_1 \neq 0$. Hence

$$E \leq \hat{E}_1.$$ \hspace{1cm} (6.32)

It is now observed that for any index $k \leq N$, there is at least one linear combination of the first $k$ eigenfunctions of $\hat{H}$ which is orthogonal to the lowest $(k-1)$ eigenfunctions of $H$. This is a consequence of the fact that the trial function in the variational method is constructed so as to be similar in class or type to the wavefunction which it approximates, and so shares the orthogonality properties of the unknown wavefunction. (Each of the eigenfunctions of $\hat{H}$ corresponds to a distinct trial function). According to Theorem 6, this linear combination of the $k$ $\hat{\psi}_i$ can be used as the trial function in the search for the $k$-th eigenvalue. For this combination of functions, inequality (6.32) holds. At the same time, Theorem 6 states that the approximate energy is higher than the actual value. Hence

$$\hat{E}_k \geq E_k \geq E'_k.$$ \hspace{1cm} (6.33)

It is now necessary to investigate what happens to the eigenvalues from the linear-variation method when the number of basis functions $m$ is increased. The easiest proof is obtained with the help of the "minimum-maximum theorem".
According to this principle, the eigenvalue $E_k$ of the Hamiltonian $H$ is found by maximising the minimum of the energy-expectation-value under the constraint that the trial function $\psi$ should be orthogonal to $(k-1)$ arbitrary functions $\omega_i$. In other words, the energy is to be minimised with respect to the trial function $\psi$, and maximised with respect to the arbitrary orthogonal functions $\omega_i$:

$$E'_k = \max_{\psi} \min_{\omega_i} \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle,$$

(6.34)

$$\langle \omega_i | \psi \rangle = 0 \text{ for } i=1,2,\ldots,k-1.$$

The minimum-maximum principle is proved by the following argument. Whatever form the $\omega_i$ take, they at most define a $(k-1)$-th dimensional linear space. Therefore, there is at least one combination of the first $k$ exact eigenfunctions of $H$ which is orthogonal to all, which can be used as a trial function. In terms of the $k$ eigenfunctions, this trial function is

$$\psi = \sum_{i=1}^{k} c_i \psi'_i.$$

(6.35)

The energy of this state is

$$E = \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle = \sum_{i=1}^{k} |c_i|^2 E'_i / \sum_{i=1}^{k} |c_i|^2.$$

(6.36)
Since \( E \) is an average, it cannot be greater than the largest energy appearing in the numerator, which is \( E'_k \). Therefore, none of the energies resulting from this trial function can be greater than \( E'_k \). Therefore, the largest minimum of the energy expectation value is always smaller than, or equal to, the \( k \)-th exact eigenvalue.

On the other hand, if the arbitrary functions \( \omega_i \) are chosen to be the exact first \( k \) eigenfunctions,

\[
\omega_i = \psi'_i, \quad \text{for } i = 1, 2, \ldots, k-1, \tag{6.37}
\]

then a trial function which is orthogonal to them is \( \psi'_k \), the \( k \)-th exact eigenfunction. The minimum of the energy expectation value from this test function is the exact energy \( E'_k \). Thus, the minimum-maximum principle exactly defines a given eigenvalue.

SECTION 6.8 - THE ACCURACY OF THE APPROXIMATE EIGENVALUES AS A FUNCTION OF NUMBER OF BASIS FUNCTIONS

The minimum-maximum principle is now employed in proving that the energies in the linear-variation method always improve in accuracy when the basis set is increased. The concept that the basis set are exact eigenfunctions of a projected Hamiltonian \( \hat{H} \) again finds application.

Let there be \( N \) linearly-independent basis functions in the set. The approximate eigenfunctions and eigenvalues of \( H \) are equal to the exact eigenfunctions and eigenvalues of \( \hat{H} \), as proved
Thus the \( k \)-th eigenvalue is \( \tilde{E}_k(N) \). The \((k-1)\)-th eigenvalue is \( \tilde{E}_{k-1}(N) \). When the basis set is increased by one member \( \phi_{N+1} \), all the eigenvalues change and in particular the \( k \)-th eigenvalue becomes \( \tilde{E}_k(N+1) \). As \( \phi_{N+1} \) is linearly independent of the first \( N \) basis functions, it can always be made orthogonal to them and hence to the trial functions for the \( N \)-dimensional space. \( \hat{\mathbf{h}} \) being a fully-fledged Hamiltonian, its eigenvalues are given by the minimum-maximum principle, so that

\[
\tilde{E}_k(N) = \min_{\psi} \max_{\omega} \langle \psi | \hat{\mathbf{h}} | \psi \rangle / \langle \psi | \psi \rangle,
\]

\[
\langle \phi_{N+1} | \psi \rangle, \langle \omega | \psi \rangle = 0, \quad i = 1, 2, \ldots, k-1;
\]

(6.38)

\[
\tilde{E}_{k-1}(N) = \min_{\psi} \max_{\omega} \langle \psi | \hat{\mathbf{h}} | \psi \rangle / \langle \psi | \psi \rangle,
\]

\[
\langle \phi_{N+1} | \psi \rangle, \langle \omega | \psi \rangle = 0, \quad i = 1, 2, \ldots, k-2;
\]

(6.39)

and

\[
\tilde{E}_k(N+1) = \min_{\psi} \max_{\omega} \langle \psi | \hat{\mathbf{h}} | \psi \rangle / \langle \psi | \psi \rangle,
\]

\[
\langle \omega | \psi \rangle = 0, \quad i = 1, 2, \ldots, k-1.
\]

(6.40)

The \( \psi \) in (6.38) - (6.40) are appropriate combinations of the basis functions. Contrary to what the notation might perhaps indicate, the three trial functions are all different from each other. In (6.38) and (6.39), \( \psi \) is expressed in terms of \( N \) basis functions while in (6.40) it is expressed in terms of \( N+1 \) of them. The variational coefficients are all different from one case to the next.

A comparison of (6.39) and (6.40) shows that the trial
functions for \( \hat{E}_{k-1}(N) \) and \( \hat{E}_k(N+1) \) are both orthogonal to \( k-1 \) functions, except that for the former, one of these functions is fixed, while for the latter it is not. According to the minimum-maximum principle, the expectation-value minimum should be maximised under the condition that the trial function should be orthogonal to the \( \omega_i \), and is clearly higher in the case which offers greater flexibility in choice:

\[
\hat{E}_{k-1}(N) \leq \hat{E}_k(N+1). \tag{6.41}
\]

Comparing now the prescriptions for \( \hat{E}_k(N+1) \) and \( \hat{E}_k(N) \), it is seen that the trial functions are orthogonal to the same number of arbitrary functions. However, there is less latitude in the choice of the trial function for the latter case because the number of basis functions is smaller. Therefore on minimising the energy expectation value with respect to the trial functions, the former case gives a lower result.

\[
\hat{E}_k(N+1) \leq \hat{E}_k(N). \tag{6.42}
\]

Inequality (6.42) gives the main result - that the energy from the linear-variation method always decreases when the basis set is increased, and therefore improves in accuracy. The result in (6.41) guarantees that no matter how many basis functions are used, the eigenvalues are still separated, ensuring that the \( k \)-th approximate eigenvalue always remains higher than the \( (k-1) \)-th
exact eigenvalue.

With the results in this chapter, the linear-variation method is put on a sound footing, and can be applied to practical problems with perfect confidence.
CHAPTER SEVEN - THE GAUSSIAN-EXPANSION METHOD

SECTION 7.1 - THE ROLE OF THE COORDINATES IN THE VARIATIONAL FORMULATION

In the last chapter, a general discussion showed how the variational method in general, and the linear-variation method in particular, may be applied to the solution of the Schroedinger equation. Implicit throughout the discussion was the importance of a judicious choice of trial function. One of the prime determinants of this is the choice of coordinates. It was mentioned in Chapter 5 how there are three ways to choose the six coordinates of the reduced problem. Any one of these choices can be used alone to prosecute the solution, as they are all simply different representations of the same thing. In fact, any two can be expressed in terms of the third, and in that sense, they are all equivalent. Despite this equivalence however, they are not all equally adapted to a particular problem. If only one channel is to be used, the physical situation which obtains in the system must be consulted before a choice can be made, as this determines which channel is most suitable. An example clarifies this observation.

Suppose one of the three particles moves faster or more
slowly than the other two, or is much farther or closer on average to the centre of mass of the system. As there are two vectors in each channel for three particles, and they are defined in an asymmetrical way, only one choice of re-arrangement coordinates is naturally designed to express this intrinsic asymmetry. This is the one in which the displacement of the odd particle is measured more uniquely than those of the other two; and by means of the parameters which define that vector, the motion of the odd particle can be especially described. If this particle is the one labelled 1, then the set of coordinates 1 in Fig. 7.1 is the correct choice.

The situation just described holds if the system lies in the domain of the Born-Oppenheimer approximation. On the other hand, if the masses are not disparate, then the wavefunction is a sum of comparable components in the coordinates of each of the three re-arrangement channels. Using only one re-arrangement channel in that case renders the expansion of the trial function unduly long, since the components in the coordinates of the other two must be effectively expressed in terms of those chosen. The series is shortened by explicitly including all three re-arrangement coordinates in the definition of the trial function. This is desirable, because the basis functions - the individual terms in the series - are rarely orthogonal. This situation may lead to near-linear dependence among them if they are many, and subsequently to difficulties in the diagonalization.

Owing to the near-parity of the kaon mass and the reduced
mass of the two protons, the ppK system should be studied by including explicitly all the re-arrangement coordinates in the specification of the wavefunction. As a matter of fact, it is possible to make do with only two without inviting undue consequence. Because two of the particles in this system are identical, two re-arrangements are similar. All the same, in the interests of generality, the case of three re-arrangement channels is analysed here.

SECTION 7.2- THE ADVANTAGES OF THE GAUSSIAN-EXPANSION METHOD

The Gaussian-expansion method of Kamimura [17,83-85] makes use in its general form of all three sets of re-arrangement coordinates. Therefore it applies to any three-body system. It is distinguished as well by a clever choice for the radial part of the wavefunction, which results in all the matrix elements which appear in the Rayleigh-Ritz method being given in closed form for potentials in power, inverse-power, Gaussian or product forms of these three.

Even though all three re-arrangement coordinates of a system are used in this calculation, the matrix elements are formally constructed by defining all the integrations in terms of a volume element in one choice of coordinates only. As the most general integrand is a function of all three sets of coordinates, this first choice is not always the most convenient for integration. Because of this, matters are contrived so that transformation of the integrand to a more useful set of re-arrangement coordinates
is easy and results in integrable functions. From this standpoint, the best coordinates for the reduced problem are the Jacobi set defined by setting $\beta_i = m_i$ (where for the channel 1 for example, $i = 2$ and 3) in (5.4). These coordinates — as their label might suggest — are so designed that the Jacobian determinant accompanying the transformation of the volume element from one choice to another is unity. This useful property means that if the original coordinates of the variable of integration by which all the matrix elements are formally defined do not appear in the integrand, the transformation to one of the other two consists of the trivial exercise of changing the volume element. It should henceforth always be understood that this has been done; all matrix elements will appear with the most convenient choice of volume element.

A second influence on the ease with which transformations of integrands might be achieved is the radial form of the trial function. Gaussian functions have been preferred to exponentials because they do indeed facilitate these transformations better.

In order to derive the matrix elements, the inter-relations among the Jacobi coordinates are necessary. In addition, the expressions of the laboratory coordinates in terms of Jacobi sets are needed in the specification of the dipole transition element.

SECTION 7.3 - THE JACOBI COORDINATES

The three possible choices of the Jacobi coordinates in terms of the coordinates of the three particles in the laboratory
system are:

For Channel 1,

\[ r_1 = x_3 - x_2, \]  
\[ R_1 = x_1 - (m_2 x_2 + m_3 x_3)/(m_2 + m_3); \]

for Channel 2,

\[ r_2 = x_3 - x_1, \]  
\[ R_2 = x_2 - (m_1 x_1 + m_3 x_3)/(m_1 + m_3); \]

and

for Channel 3:

\[ r_3 = x_1 - x_2, \]  
\[ R_3 = x_3 - (m_1 x_1 + m_2 x_2)/(m_1 + m_2). \]

For each choice,

\[ X = (m_1 x_1 + m_2 x_2 + m_3 x_3)/(m_1 + m_2 + m_3). \]

The various vectors are illustrated in Fig. 7.1.
Fig. 7.1. The re-arrangement Jacobi coordinates of the three-body system.
SECTION 7.4 - THE LABORATORY DISPLACEMENTS IN TERMS OF THE JACOBI COORDINATES

The laboratory coordinates together with the transformed Hamiltonians for the internal motion of the system (all fully derived in Appendix A) are:

For channel 1,

\[ H_1 = -\left(\frac{\hbar^2}{2\mu_1}\right)\dot{x}_1^2 - \left(\frac{\hbar^2}{2M_1}\right)\dot{R}_1^2 + V(r_1, R_1), \]  
\[ x_1 = X + (m_2 + m_3)R_1/M, \]  
\[ x_2 = X - m_1 R_1/M - m_3 r_1/(m_2 + m_3), \]
and
\[ x_3 = X - m_1 R_1/M + m_2 r_1/(m_2 + m_3). \]

where

\[ M = m_1 + m_2 + m_3, \]  
\[ 1/\mu_1 = 1/m_2 + 1/m_3, \]

and

\[ 1/M_1 = 1/m_1 + 1/(m_2 + m_3). \]

For Channel 2,

\[ H_2 = -\left(\frac{\hbar^2}{2\mu_2}\right)\dot{x}_2^2 - \left(\frac{\hbar^2}{2M_2}\right)\dot{R}_2^2 + V(r_2, R_2), \]
\begin{align}
  x_1 &= X - m_2 R_2 / M - m_3 r_2 / (m_1 + m_3), \\
  x_2 &= X - (m_1 + m_3) R_2 / M, \\
\end{align}

and

\begin{align}
  x_3 &= X - m_2 R_2 / M + m_1 r_2 / (m_1 + m_3), \\
\end{align}

where

\begin{align}
  1 / \mu_2 &= 1 / m_1 + 1 / m_3, \\
\end{align}

and

\begin{align}
  1 / M_2 &= 1 / m_2 + 1 / (m_1 + m_3), \\
\end{align}

Finally, for Channel 3;

\begin{align}
  H_3 &= - \left( \frac{\hbar^2}{2\mu_3} \right) \nabla_{R_3}^2 - \left( \frac{\hbar^2}{2M_3} \right) \nabla_{r_3}^2 + V(r_3, R_3), \\
  x_1 &= X - m_3 R_3 / M + m_2 r_3 / (m_1 + m_2), \\
  x_2 &= X - m_3 R_3 / M - m_1 r_3 / (m_1 + m_2), \\
\end{align}

and

\begin{align}
  x_3 &= X + (m_1 + m_3) R_3 / M, \\
\end{align}

where
\[ \frac{1}{\mu_3} = \frac{1}{m_1} + \frac{1}{m_2}, \quad (7.25) \]

and

\[ \frac{1}{M_3} = \frac{1}{m_3} + \frac{1}{(m_1 + m_2)}. \quad (7.26) \]

SECTION 7.5 - THE INTER-RELATIONS AMONG THE JACOBI COORDINATES

The three sets of coordinates are, as mentioned above, expressible in terms of one another. In anticipation of future use, these inter-relations are now given.

\[ r_1 = m_1 r_2/(m_1 + m_3) - R_2, \quad (7.27) \]

\[ R_1 = - m_3 M r_2/[(m_2 + m_3)(m_1 + m_3)] - m_2 R_2/(m_2 + m_3), \quad (7.28) \]

\[ r_1 = m_1 r_3/(m_1 + m_2) + R_3, \quad (7.29) \]

\[ R_1 = m_2 M r_3/[(m_1 + m_2)(m_2 + m_3)] - m_3 R_3/(m_2 + m_3), \quad (7.30) \]

\[ r_2 = m_2 r_1/(m_2 + m_3) - R_1, \quad (7.31) \]

\[ R_2 = - m_3 M r_1/[(m_1 + m_3)(m_2 + m_3)] - m_1 R_1/(m_1 + m_3), \quad (7.32) \]

\[ r_2 = - m_2 r_3/(m_1 + m_2) + R_3, \quad (7.33) \]

\[ R_2 = - m_1 M r_3/[(m_1 + m_3)(m_1 + m_2)] - m_3 R_3/(m_1 + m_3), \quad (7.34) \]

\[ r_3 = m_3 r_1/(m_2 + m_3) + R_1, \quad (7.35) \]
\[ R_3 = m_2 r_1 / [(m_1 + m_2)(m_2 + m_3)] - m_1 R_1 / (m_1 + m_2), \]  
(7.36)

and

\[ r_3 = -m_3 r_2 / (m_1 + m_3) - R_2, \]  
(7.37)

\[ R_3 = m_1 M r_2 / [(m_1 + m_2)(m_1 + m_3)] - m_2 R_2 / (m_1 + m_2). \]  
(7.38)

Relations (7.27) - (7.38) are readily obtained by equating the two expressions for \( x \), in the two coordinate systems under consideration.

SECTION 7.6 - SPECIFICATION OF THE WAVEFUNCTION

The main quantity of interest in this calculation is the energy. The states for which it is sought are identified by the quantum numbers for conserved quantities whose operators commute with the Hamiltonian. These operators are the ones which serve to differentiate the states and confer on them their class, as discussed in Chapter 6. In a many-body system, the most important such quantity is the total spin \( J \). Its component \( m \) in the direction of externally-applied magnetic fields is an auxiliary label whose importance increases if the potential is a function of the angular coordinates of inter-particle vectors. Both numbers are used to label the classes of solution here.

According to the discussion in Chapter 6, the number of solutions to the energy equals the number of basis functions. Thus, apart from the two explicitly introduced in the trial function, there is a third quantum number. In three-body theory,
this quantum number is labelled \( v \), and is called the vibrational quantum number. It is evidently analogous to the principle quantum number \( n \) which occurs in two-body theory. In many numerical solutions of the Schroedinger equation for two-body systems, the problem is specified in terms of the angular-momentum quantum numbers which appear in the kinetic operator, (and possibly in the potential if it is not spherically symmetric), and \( n \) is assigned to the resultant energy solutions by looking at the magnitudes. The vibrational quantum number appears, and is treated, in the same way here.

The wavefunction on which the transformed Hamiltonians (the derivation of which is given in Appendix A) operate is denoted \( \Psi_{JM'} \). As there are two vectors involved in the coordinate system, \( J \) is composed by vectorial addition of the angular momenta associated with them. The angular momenta are respectively \( l_a \) and \( L_a \) for the coordinates \( r_a \) and \( R_a \) \((a=1,2,3)\), so that

\[
J = l_a + L_a. \tag{7.39}
\]

The interactions among the three particles are central, and therefore, the angular wavefunctions proper to \( l_a \) and \( L_a \) are the spherical harmonics \( Y_{l_a} (r_a) \) and \( Y_{L_a} (R_a) \). Thus for the channel \( a \), the angular part of the wavefunction is given by

\[
Y_{JM}(r_1, r_2, R) = [Y_{l_a} (r_a) \otimes Y_{L_a} (R_a)]_{JM}, \tag{7.40}
\]

where \([ \ldots \otimes \ldots ]_{JM} \) denotes the tensor product \([110,111] \)
In (7.41), $m_l$ and $m_a$ are the magnetic quantum numbers for $l_a$ and $L_a$, while $(^1_m l_a l_m | J^M)$ is a Clebsch-Gordan coefficient.

The radial part of the wavefunction is what the Rayleigh-Ritz method helps to determine.

SECTION 7.7 - THE TRIAL FUNCTION

Naturally, the angular part of the trial wavefunction is given by (7.40). The radial form is chosen on the grounds of convenience in calculating the matrix elements in the diagonalization problem and is, for a channel $a$ [17,83-85], given by

$$R(r_a, R_a) = N_a r^l_a R^l_a \exp(-\nu r^2) \exp(-\lambda R^2).$$

(7.42)

where $N_a$ is a normalization factor such that

$$\int_0^\infty \int_0^\infty R_a^2 r^2 dr_a R_a^2 dR_a = 1.$$  

(7.43)

The quantities $r_a$ and $R_a$ are simply the magnitudes of the vectors $r_a$ and $R_a$ respectively. The expression for $N_a$ is
To connect with the earlier discussion concerning the role of the various re-arrangement coordinates, the trial function may be viewed symbolically as

$$\Psi_t = \sum_{i=1}^{3} \sum_{j=1}^{\text{max}} (r_i, R_j).$$  

(7.45)

Explicitly, it is given by

$$\Psi_t = \sum_{a=1}^{3} \sum_{i=1}^{\text{max}} \sum_{j=1}^{\text{max}} N_{1a}^{(i)j} C_{1a}^{(i)j} r_a R_a \exp(-\nu r_a^2)$$

$$\times \exp(-\lambda R_a^2)[Y_{1a}^{(r_a)} \otimes Y_{1a}^{(R_a)}]_{JM'}$$

(7.46)

where $C_{1a}^{(i)j}$ is the variational coefficient.

The various summations in (7.46) give added flexibility in the radial part of the trial function. Thus, the $i$- and $j$-summations improve the extent to which the radial part of the actual solution is approximated by associating to each value of $l_a$ and $L_a$ several Gaussian functions. This is important since the Gaussian is clearly not the optimum form for the second factor of the radial dependence. A first analysis recommends the exponential form, which naturally arises in the exact treatment of hydrogen-like systems. The exponential would be a superior choice if the fact that some matrix elements would have to be evaluated numerically was not a consideration. The Gaussians allow all the matrix elements to be given in closed form for the basic problem.
of Coulombic interactions only, and this is such a great advantage that their slightly inferior suitability is overlooked.

The role of \( \nu \) and \( \lambda \) in shaping the wavefunction is better appreciated when they are written in the forms

\[
\nu_i = \frac{1}{r_i^2} \quad \text{(7.47)}
\]

and

\[
\lambda_j = \frac{1}{R_j^2} \quad \text{(7.48)}
\]

they are obviously related to the size of the ion. They are the ones which change as \( i \) and \( j \) run through their ranges. For a given combination of \( \nu \) and \( \lambda \) in the series (7.46), \( r_i \) and \( R_j \) are chosen from minimum values (for which \( i=1, j=1 \)) to maximum values (for which \( i=i_{\text{max}}, j=j_{\text{max}} \)) in such a way that the \( r_i \) and the \( R_j \) are in geometrical progression. The limits and the number of terms in the geometric progressions are determined from experience or by trial and error, and are input parameters of the calculation.

The summations over \( \nu \) and \( \lambda \) are specified by simply selecting combinations \( (\nu, \lambda) \) which satisfy the rules of angular-momentum algebra. These combinations are selected for one re-arrangement channel at a time, and as has already been stated, each one has an \( i- \) and a \( j- \)series associated with it. For a given value of \( j \), the angular momenta \( \nu \) and \( \lambda \) satisfy the conditions
and

\[ (-1)^J = (-1)^{1a + L_a}. \]  

(7.50)

It is a straightforward task to compute the total number of basis functions. The number of terms in each re-arrangement channel is the sum over all \((1_a, L_a)\) combinations of the product of the total number of terms in sums over \(i\) and \(j\). To give an example - if \(J=0\), the combinations \((1_a, L_a) = (0,0), \text{and} (1,1)\) might be chosen for each of the three re-arrangement channels. If the \(i\)- and \(j\)-summations in every one of the six combinations of \((1_a, L_a)\) have five terms each, there are \(5 \times 5 + 5 \times 5 = 50\) basis functions in each channel, and 150 altogether.

Before eq. (7.46) is used in the linear-variation method, the series has to be ordered so that each of the basis functions is identified by one index

\[ k = k(a, i, j, 1_a, L_a) \]

which runs from 1 to \(N\), where \(N\) is their total number. Each such term is

\[ \phi_k = \mathcal{N}^{(1_a, L_a)} r_a^{1a} R_{a}^{L_a} \exp(-\nu \ r_a^2) \exp(-\lambda_j R_{a}^2) Y_{1a} (\hat{r}_a) Y_{L_a} (\hat{R}_a) J_{JM}, \]

(7.51)

and

\[ 1_a + L_a \leq J \leq |1_a - L_a|, \]

(7.49)
\[ \Psi_t = \sum_{k=1}^{N} c_k \phi_k, \]  

(7.52)

where

\[ c_k = \mathcal{C}_{i,j}^{a,a,La}. \]  

(7.53)

SECTION 7.8 - THE EXPRESSIONS FOR THE MATRIX ELEMENTS

The generalised matrix eigenvalue equation which yields the eigenvalues and the variational coefficients is given by eq. (6.19). In this section, the matrix elements which appear in that equation are given. The principles by which each one is derived from the trial function defined in eq. (7.46) are the same, and it would serve no didactic purpose to minutely derive each one. The necessary techniques are illustrated by detailed consideration of just one of the matrix elements, which exercise is pursued in Appendix B. Here, the final results [85] are simply quoted.

In the following expressions, a simplified notation is used to avoid untidiness. All the quantities proper to a basis function \( \phi_k \) are characterised by the label of the coordinates \( a \). This notation is sufficient, and introduces no confusion because the matrix elements will be given in terms of two basis functions at a time. The general matrix element involves one set of coordinates in the bra, another in the ket, and a third set in the operator, and all parameters are completely specified in terms of the coordinate labels.
The matrix element for the overlap of two basis functions is

\[
O_{kk'} = \langle \phi_k^{(a)} | \phi_{k'}^{(b)} \rangle = (-1)^j N_N \sum_{a'b} \langle 1'L'_{j'} | 1'L_{j} \rangle a'a'b \rightarrow a'a'a'a \\
\times \sum_{\lambda=0}^{\Lambda} (1|0\lambda0)_{a'a} (1|0\lambda0)_{a'a} W(1|a'a'a'a;\Lambda\omega) \\
\times \frac{\pi^A}{4} \frac{(2m+2\lambda+1)!}{2n^m+n^\lambda+2} \frac{\xi^{n-m}}{(\eta\xi-\xi^2)^{n^\lambda+3/2}} \\
\times \sum_{k=0}^{m} \frac{(2k+2\lambda+2n+1)!}{(2k+2\lambda+1)!} \left( \begin{array}{c} m \\ k \end{array} \right) \left( \frac{\xi^2}{\eta\xi-\xi^2} \right)^k. \tag{7.54}
\]

The Raynal-transformation coefficient is given by \([112,113]\)

\[
\langle 1'L'_{j'} | 1'L_{j} \rangle a'a'b \rightarrow a = (21\rightarrow 1)(21\rightarrow 1) \\
\times \sum_{\mu=0}^{1 \rightarrow -\mu} \gamma_{ba}^{L_\mu} \gamma_{ba}^{L_\mu} \delta_{ba}^{\mu} \delta_{ba}^{\mu} (1_{-\mu0L_{b}+T+\mu0 \rightarrow 10})_{a} (\mu0T_{a}-\mu0 | L'_{a}) \\
\times \left[ \begin{array}{c} 21_b \\ 2\mu \\ 2(T-\mu) \end{array} \right]^{1/2} \left[ \begin{array}{c} 1_{-\mu}^{L_\mu} \\ \mu \rightarrow T+\mu \\ \mu \rightarrow T-\mu \end{array} \right] \\
\times \left[ \begin{array}{c} 1_{-\mu}^{L_\mu} \\ \mu \rightarrow T+\mu \\ \mu \rightarrow T-\mu \end{array} \right]^{1/2} \\
\times \left[ \begin{array}{c} 1_{b}^{L_\mu} \\ \mu \rightarrow L_{b}^{T-\mu} \\ \mu \rightarrow L_{b}^{T+\mu} \end{array} \right]^{1/2} \\
\times \left[ \begin{array}{c} 1_{b}^{L_\mu} \\ \mu \rightarrow L_{b}^{T-\mu} \\ \mu \rightarrow L_{b}^{T+\mu} \end{array} \right]^{1/2} \\
\times \left[ \begin{array}{c} 1_{b}^{L_\mu} \\ \mu \rightarrow L_{b}^{T-\mu} \\ \mu \rightarrow L_{b}^{T+\mu} \end{array} \right]^{1/2} \tag{7.55}
\]

where as usual

\[
\left[ \begin{array}{c} a \\ b \end{array} \right] = a!/(a-b) \ b! , \tag{7.56}
\]

and the nine-argument braces stand for the nine-j symbol.

In expression (7.54) \( W \) stands for the Racah coefficient, and \( \hat{l} = (2l+1)^{1/2} \), for example.

The quantities \( \gamma_{ba}^{L_\mu} \), \( \gamma_{ba}^{L_\mu} \), \( \delta_{ba}^{\mu} \) and \( \delta_{ba}^{\mu} \) define the coordinates \((r_b^R_a, R_b^R_a)\) in terms of the coordinates \((r_a^R, R_a^R)\) and come from the relations (7.27) to (7.38). Thus
\[ r_b = \gamma_{ba} r_a + \delta_{ba} R_a , \tag{7.57} \]

and

\[ R_b = \gamma'_{ba} r_a + \delta'_{ba} R_a . \tag{7.58} \]

while \( \eta, \zeta \) and \( \xi \) have the definitions

\[ \eta = \nu_a + \nu \gamma^2_{ba} + \lambda b_{ba} , \tag{7.59} \]
\[ \zeta = \lambda a + \nu \delta^2_{ba} + \lambda b_{ba} , \tag{7.60} \]

and

\[ \xi = \nu b_{ba} \delta_{ba} + \lambda b_{ba} \delta'_{ba} . \tag{7.61} \]

The other quantities are

\[ m = (\lambda_a + \tau - \lambda)/2 , \tag{7.62} \]

and

\[ n = (\lambda_a + \lambda_b + \lambda - \tau + \lambda)/2 . \tag{7.63} \]

The summation ranges for the various indices are determined by the Clebsch-Gordan coefficients through the triangle inequality [106]. Thus
\[ 1_a + 1'_a \geq \lambda \geq \left| 1_a - 1'_a \right|, \tag{7.64} \]
\[ L_a + L'_a \geq \lambda \geq \left| L_a - L'_a \right|, \tag{7.65} \]
\[ 1_b + L_b - T \geq 1_a \geq \left| L_a - T + 2\mu - 1_b \right|, \tag{7.66} \]
\[ T \geq L'_a \geq \left| T - 2\mu \right|, \tag{7.67} \]

and from the angular part of the wavefunction when \( j \) is composed from \( 1_a \) and \( L_a \),
\[ 1_a + L_a \geq j \geq \left| 1_a - L_a \right|. \tag{7.68} \]

The matrix elements involving the Hamiltonian operator are best expressed by taking the interaction and the kinetic-energy parts separately. For the interaction \( V(r_c) \), the matrix element with respect to the the basis functions \( \phi_k(a) \) and \( \phi_{k'}(b) \) is

\[
\langle \phi_k(a) | V(r_c) | \phi_{k'}(b) \rangle = (-1)^j N_a N_b \sum_{l_a l'_a j} \langle l'_a l_a j \rangle \langle 1_a l_a j | V(r_c) | \phi_{k'}(b) \rangle =
\]
\[
\times \sum_{b c} \langle 1_b L_b c | V(r_c) | 1_c L_c b \rangle \langle 0 \rangle \langle \lambda_0 | V(r_c) | \lambda_0 \rangle
\]
\[
\times W(1, 1', \lambda, \lambda) \frac{\sqrt{\pi}}{4} \left( \frac{\xi^\lambda}{\zeta^{m+\lambda+3/2}} \right) (2m+2\lambda+1)!!
\]
\[
\times \sum_{k=0}^{m} \left( \frac{2\xi^2}{\zeta} \right)^k \binom{m}{k} U(r_c), \tag{7.69} \]

where

\[
U(r_c) = \int_0^\infty V(r_c) r_c^{2n+\lambda+K+1} \exp(-\theta r_c^2) dr_c. \tag{7.70} \]

For the Coulomb potential \( V = 1/r_c \), \( U \) is [108]
\[ U(r) = \frac{(n+\lambda+k)!}{2(n-\xi^2/\zeta)^{n+\lambda+k+1}}. \]  

(7.71)

and for the Gaussian potential \( V = \exp(-\mu r^2) \),

\[ U(r) = \frac{(2(n+\lambda+k)+1)!}{2(2(n-\xi^2/\zeta+\mu))^{n+\lambda+k+1}} \frac{(\pi/(n-\xi^2/\zeta+\mu))^{1/2}}{2(n-\xi^2/\zeta+\mu)^n} \]  

(7.72)

Here, \( m \) and \( n \) are defined differently from previously, and are now

\[ m = (\tau + \tau' - \lambda)/2, \]  

(7.73)

and

\[ n = (\tau_a + \tau_b + \lambda - \tau - \tau' - \lambda)/2 \]  

(7.74)

also

\[ \eta = \nu \gamma^2 + \lambda \gamma' \delta^2 + \nu \gamma^2 + \lambda \gamma' \delta^2, \]  

(7.75)

\[ \zeta = \nu \delta^2 + \lambda \delta' \delta^2 + \nu \delta^2 + \lambda \delta' \delta^2, \]  

(7.76)

\[ \xi = \nu \gamma \delta + \lambda \gamma' \delta' + \nu \gamma \delta + \lambda \gamma' \delta'. \]  

(7.77)

From the inequalities

\[ l_c + l'_c = \lambda \geq |l_c - l'_c|, \]  

(7.78)

\[ l_c + l'_c = \lambda \geq |l_c - l'_c|, \]  

(7.79)
\begin{align}
L_c \geq J \geq |L_c - L_c|,
\tag{7.80}
\end{align}

\begin{align}
L_c' \geq J \geq |L_c' - L_c|,
\tag{7.81}
\end{align}

\begin{align}
L_a - L \geq J \geq |L_a - L_a + 2\lambda|,
\tag{7.82}
\end{align}

\begin{align}
L_b - L' \geq J \geq |L_b - L_b + 2\lambda'|,
\tag{7.83}
\end{align}

\begin{align}
\tau \geq L_c \geq |\tau - 2\lambda|
\tag{7.84}
\end{align}

and

\begin{align}
\tau' \geq L_c' \geq |\tau' - 2\lambda'|
\tag{7.85}
\end{align}

come the summation ranges. Inequalities (7.80) to (7.83) come from the Clebsch-Gordan coefficients in the Raynal-transformation coefficients.

Finally, the kinetic matrix element is

\begin{align}
\langle \phi_k(a) | (-\hbar^2 \nabla^2 / 2\mu) \mathcal{R}_{a,b} | \phi_k'(b) \rangle = (-1)^J N_a N_b 
\sum_{a,b} \langle L \ L' \ J \ | 1 
\sum_{a,b} \langle L \ L' \ J \ | 1 
\sum_{a,b} \langle L \ L' \ J \ | 1 
\sum_{a,b} \langle L \ L' \ J \ | 1 
\sum_{a,b} \langle L \ L' \ J \ | 1
\tag{7.86}
\end{align}

where

\begin{align}
I_1 &= \tilde{Q} - \pi \frac{\xi^\lambda}{\xi_{m_i} + \lambda + 3/2} \left( \frac{2m_i + 2\lambda + 1}{2} \right)^{n_i} \left( \frac{\eta\zeta - \xi^2}{\eta\zeta - \xi^2} \right)^{n_i + \lambda + 3/2} \\
&\times \sum_{k=0}^{m_i} \frac{(2k + 2\lambda + 2n_i + 1)!}{(2k + 2\lambda + 1)!} \left( \frac{m_i}{k} \right) \left( \frac{\xi}{\eta\zeta - \xi^2} \right)^k
\tag{7.87}
\end{align}

with
\[ Q_1 = 2h^2(\frac{1}{a} + 3/2)/m_a + 2h^2(\frac{1}{a} + 3/2)/M_a, \]  
(7.88)

\[ n_1 = (\frac{1}{a} + \tau - \lambda)/2 \]  
(7.89)

\[ Q_2 = -2h^2 \nu_a^2/m_a, \]  
(7.90)

\[ m_2 = (\frac{1}{a} + \tau - \lambda)/2, \]  
(7.91)

\[ n_2 = (\frac{1}{a} + \nu_a^2 - \tau - \lambda + 2)/2; \]  
(7.92)

\[ Q_3 = -2h^2 \lambda_a^2/M_a, \]  
(7.93)

\[ m_3 = (\frac{1}{a} + \tau - \lambda + 2)/2, \]  
(7.94)

\[ n_3 = (\frac{1}{a} + \nu_a^2 - \tau - \lambda)/2. \]  
(7.95)

and

The summation ranges are the same as for the case of the overlap matrix elements. So are the definitions of \( \eta, \xi \) and \( \zeta \).

SECTION 7.9 - EXPECTATION VALUES

Once the stationary points of expression eq. (6.1) have been obtained, the variational coefficients \( c_k \) in the expansion for the wavefunction eq. (7.52) are known, and the computation of expectation values can proceed. It should be noted that a wavefunction which gives an energy of given accuracy is itself less accurate, since according to eq. (6.10), the energy quadratically converges to the exact value, while the convergence of the wavefunction is only linear. Thus expectation values are obtained less accurately than the corresponding energy.
Several expectation values are of direct physical interest. The length of the kaonic bond between the two protons is given by the expectation value of the separation \( r_3 = |r_3| \) (as shown in Fig. 7.1). A second measure of the size of the ion is the square root of the expectation value of \( r^2 \). Yet a third is the expectation value of \( r_1 \); being the average distance of the kaon from a proton, it gives the position of the maximum density of the kaon charge distribution. A collection of these expectation values for various three-body ions is given in reference [114].

SECTION 7.10 - THE EXPRESSIONS FOR THE EXPECTATION VALUES

As the wavefunction is given by

\[
\psi_{JM} = \sum_{k=1}^{M} c_k \phi_k,
\]

the expectation value for the operator \( O \) is

\[
\langle O \rangle = \frac{\sum_{k, k'} c_k^* c_{k'} <\phi_k | O | \phi_{k'}>}{\sum_{k, k'} c_k^* c_{k'} <\phi_k | \phi_{k'}>}
\]

For \( O = r_c^q \), the matrix elements are identical to those for the interaction term in the Hamiltonian (which is carefully derived in Appendix B). For this reason, they are given by (B41), with

\[
U(r_c) = \int dr_c r_c^{2n+q} \exp(-\eta/c^2/\xi) \]

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where

\[ 2n = l^a + l^b + 1^b + \tau - \tau' + 2k + 2 + \lambda, \quad (7.100) \]

with \( n \) a positive integer. From formulas (B45) and (B46),

\[
U(r_c) = \frac{(2n+q-1)!!}{2[2(\eta-\xi^2/\zeta)]^{n+q/2}} \left[ \frac{\pi \zeta}{\eta \zeta - \xi^2} \right]^{1/2}, \text{ if } q \text{ is even,} \quad (7.101)
\]

and

\[
U(r_c) = \frac{(n+[q-1]/2)!}{2[(\eta-\xi^2/\zeta)]^{n+[q-1]/2}}, \text{ if } q \text{ is odd.} \quad (7.102)
\]

The matrix element in the square of the wavefunction in the denominator of eq. (7.102) is evidently given by expression (7.54).
SECTION 8.1 - PRELIMINARY COMMENTS

In this chapter, the use of the computer codes based on the formulas given in Chapter 7 is explained, and the results of the calculational efforts are presented. The computer program used to obtain the energies was a modification of a basic code supplied by Kamimura, while the codes for the calculation of the matrix elements appearing in the expectation were based loosely on the main one. All calculations were carried out in double-precision arithmetic on the Prime 750 computers at the University of Surrey and the Cray 6 computer at the Rutherford-Appleton Laboratory.

The labour invested on the energy in a calculation on the ppK ion is doubled by the necessity to compute, for a given state, the energy corresponding to the full potential on the one hand, and the value for the case of no strong interaction on the other. The purely electromagnetic energy has to be subtracted from the full value for the effects of the strong interaction to manifest themselves.

SECTION 8.2 - THE STRONG INTERACTION

The strong interaction is introduced into the calculation straightforwardly by computing its matrix elements and adding them to the Hamiltonian matrix elements (6.21). A more ambiguous issue
concerns the form to be used to represent the potential. The strong force between each proton and the kaon operates in its purest form in kaonic hydrogen. But there is as yet no unanimity in the literature on the scale of strong-interaction effects in that atom [20-23]. In the absence of better guidance, convenience is consulted and the Kp potential of Deloff and Law [24] is adopted. Its Gaussian form is well suited to the present formulation, since the advantage of closed matrix elements is preserved. In the expression

\[ V_s = -(V_R^* + iV_I) \exp(-0.4586r^2/\beta^2), \quad (8.1) \]

\( V_R \) and \( V_I \) are the real and imaginary strengths and are constants for a given value of \( \beta \). The three parameters are fitted to scattering data. The values used are

\[ V_R = 526.20 \text{ MeV}, \]
\[ V_I = 429.51 \text{ MeV}, \]
\[ \beta = 0.45. \quad (8.2) \]

The matrix element of \( V_s \) is expressed by formula (7.69), with \( U \) being now given by expression (7.72).

SECTION 8.3 - DESCRIPTION OF THE INPUT DATA

Table 8.1 is an example of the input to the variational code for a calculation. The lines of input have the following meanings:
Table 8.1. Example input for energy calculation; the significance of the entries is given in the text.

<table>
<thead>
<tr>
<th>5</th>
<th>1.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>NC=2 J=0</td>
<td>1</td>
</tr>
<tr>
<td>1 0 0</td>
<td>10 18. 700. 10 20. 900.</td>
</tr>
<tr>
<td>3 0 0</td>
<td>10 20. 500. 10 20. 800.</td>
</tr>
</tbody>
</table>

Table 8.2. Strong-interaction input parameters; the identity of the entries is discussed in the text.

<table>
<thead>
<tr>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.265 526.20 429.51</td>
</tr>
</tbody>
</table>

---

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The first number on the first line selects the three-body ion of interest from the several which the general code can handle. The second number offers the possibility of constructing three-body ions in which the negative particle has an arbitrary mass. This mass is achieved by simply multiplying the appropriate negative-particle mass by the number. For normal purposes therefore, and for a given generalized hydrogen molecular ion, this factor is unity. This provision may be somewhat obscure but the need for it becomes clear later.

The correspondence between first number and molecular ion is

1 - proton-proton-muon system,
4 - proton-proton-pion system,
5 - proton-proton kaon system

and

6 - proton-proton-electron system.

The first entry on line 2 gives the number of \( (1_a, L_a) \) combinations to be used in the trial function; in combination with the channel label \( a \), these will henceforth be called configurations. The second entry is obviously the \( J \) quantum number of the state under consideration, while the third entry is the vibrational quantum number \( v \). Label \( v \) is read in to specify which of the \( N \) sets of variational coefficients is to be written out for use in computing expectation values. In many cases, only the \( v=0 \) state is bound \[115\].

In the example input, two configurations are used in the wavefunction. Line 3 gives the parameters characterising the
first one. The first entry here is the label of the Jacobi channel $a$ to which this configuration belongs. The next entries are the angular momenta $\ell_a$ and $a$ respectively. The fourth number gives the number of terms $n_i$ over the $i$-summation. Next are the values of $r_{\text{min}}$ and $r_{\text{max}}$ respectively (these parameters are defined by eq. (7.47)). The seventh entry is the number of terms $n_j$ in the $j$-summation, while the last two entries are the extremes of the size parameter for this summation, $R_{\text{min}}$ and $R_{\text{max}}$ (defined by eq. (7.48)). The number of basis functions corresponding to this configuration is the product of the fourth and the seventh entries. In the example, this number is 100, for line 3.

Line 4 has the same interpretation as line 3; the total number of basis functions in the example is 200.

Table 8.2 gives the input data for the parameters of the strong interaction. For added flexibility, there is provision for any number of Gaussian terms in the expression. This total is declared on the first line. The subsequent lines each give the exponent, which in this case is $0.4586/\beta^2$, and the strengths of the real and imaginary parts respectively.

SECTION 8.4 - GENERAL COMMENTS ON THE CALCULATIONS

In a practical calculation, the configurations are introduced systematically. First, only one is employed; the variables (the numbers of terms in the summations and the limits of the size parameters) are adjusted until the energy is as low as possible. Then another configuration makes its appearance and the process is repeated. This goes on until the energy is constant to
the desired accuracy. It is found that the various adjustables are almost independent of one another, which considerably shortens the time it takes to stabilise the energy value.

In choosing combinations of \( (l_a, l_a) \) to feed into the calculation, the smallest values consistent with the triangle inequality should always be used initially, since the importance of higher values rapidly diminishes. It is unlikely that either one of the angular momenta would need to exceed the value 2.

One of the results in Chapter 6 might seem to offer a way out of adjusting the parameters, and thereby of expediting the energy calculation. The linear-variation energy improves when the number of basis functions is increased. Thus the problem should be solvable at a stroke by using an arbitrary combination of size parameters and a very large number of basis functions. In reality, the numerical difficulties adverted to in the same chapter, which arise if the basis functions suffer from near-linear dependence, prevent this shortcut. While Gaussian functions and different powers of \( r \) or \( R \) are linearly-independent in theory, they are not always so from a numerical point of view. More importantly, if the values in some rows or columns of the Hamiltonian matrix are similar - which may happen if there are too many basis functions in a size-parameter interval - then that matrix may be ill-conditioned with respect to diagonalization of the eigenvalue problem. To prevent this, much care has to be exercised in the choice of the non-variational parameters. It is good practice to keep the number of basis functions for any configuration to the minimum consistent with requirements. Fortunately, numerical problems usually betray themselves
conspicuously by the sudden appearance of negative numbers of very large magnitude.

It is found that the channels 1, 2 and 3 do not contribute equally to the binding energy for the same combination \( (_{1a} l_a) \). Channels 1 and 2 have a bigger influence than channel 3. This circumstance can be explained from the considerations at the beginning of Chapter 7. Thus, the combination in which the angular momentum relative to a proton and the kaon is given explicitly, as in channels 1 and 2 is natural, since it suggests a conformation of particles wherein the ion is formed by the association of a second proton to kaonic hydrogen. On the other hand, it is less suitable to define an angular momentum explicitly with respect to two protons because they are never bound in the absence of a negative particle. The unequal importance of the three channels dictates that the first configuration in the systematic construction of the wavefunction should always belong to channel 1 or 2. Here it should be mentioned that though the cause of generality was served in Chapter 7 by analysing a case where all three re-arrangement channels of the three-body system figured, the computer code exploits the fact that channels 1 and 2 are identical by omitting the second. No configurations are ever entered for that channel, and it is channel 1 to which the configuration on line three of the input should always belong.

Once the energy has been obtained, the variational coefficients are known, and the expectation values can be computed. In Chapter 7, it was mentioned that in the course of the energy calculation, the basis functions are each given one index to label them when the matrix elements are compiled. The
wavefunction is extracted from the calculation by writing out the parameters for the chosen vibrational state into two files. Into the first one goes the index \( k \), and the variational coefficients for the basis functions. The second file receives the non-variational parameters, which for an index \( k \) are the channel \( a \) to which a basis function belongs, the value of \( \gamma_a \), the value of \( \nu_a \), the value of \( \lambda_a \) and the value of \( \nu_a \). The two files are then read by the program for the expectation value.

Checks on the accuracy of the calculations were made by reproducing some energy values privately communicated by Dr Kamimura [85], and then computing the energies of exotic-atom hydrogen molecular ions already treated in the literature [59,115].

SECTION 8.5 - THE VALUES OF THE CONSTANTS USED IN THE CALCULATION

The following values of constants have been used in this calculation:

\[
\begin{align*}
\pi &= 3.141592653589793, \\
\alpha &= 1/137.035982, \text{ the fine-structure constant}. \\
\hbar c &= 197.32858 \text{ MeV.F, the product of Planck's constant and the speed of light.} \\
m_e &= 0.5110034 \text{ MeV/c}^2, \text{ the electron mass.} \\
m_\mu &= 105.65948 \text{ MeV/c}^2, \text{ the muon mass.} \\
m_p &= 938.2796 \text{ MeV/c}^2, \text{ the proton mass.} \\
m_\pi &= 139.580 \text{ MeV/c}^2, \text{ the pion mass.} \\
m_K &= 493.78 \text{ MeV/c}^2, \text{ the kaon mass.}
\end{align*}
\]
The ground state of the ppK ion is the $j=0, v=0$ state. The absolute energy of this state is simply the number obtained from diagonalizing the matrix eigenvalue equation (6.19). This is not the true binding energy however, since to destroy the three-body system it is necessary only to detach one of the protons. The amount of energy which effects this is just the difference between the absolute energy and the binding energy of the 1s state in kaonic hydrogen - this atom being the residual system. It is this difference which is quoted here. Two values are used for the 1s energy. The simple result

$$E_{1s} = -Z\mu^2 e^4/2\hbar^2,$$

from the Bohr formula (here $\mu$ is the reduced mass and $Z$ the atomic number) applies when the electromagnetic energy of a ppK state is under consideration. When the total binding energy is sought, the threshold value includes the kaonic-hydrogen 1s strong-interaction shift. Unfortunately, the contribution of the 1s shift to the threshold value is attended with the uncertainties to which this quantity is subject. In addition, the usual small corrections to atomic-state energies are theoretically necessary [117]; here they are ignored because the three-body calculation is not refined.
enough to warrant their inclusion. It is enough to observe that so long as the threshold energy is quoted when the ppK binding energies are given, the original absolute values can always be reclaimed.

The threshold energies are

\[ \varepsilon_{1s} = 8614.0 \text{ keV (without the strong-interaction shift),} \quad (8.4) \]

and

\[ \varepsilon_{1s}^{(s^1)} = 9014.4 \text{ keV (with the strong-interaction shift).} \quad (8.5) \]

When the ppK energy is complex, the imaginary part is adopted without adjustment and gives the absorption rate of the kaon on the protons. The connection between the imaginary part \( E_I \) of the eigenvalue and the absorption width \( \Gamma \) is

\[ \Gamma = -2E_I. \quad (8.6) \]

As prescribed in Chapter 6, the energy from the variational method is accepted when the plot of energy against number of basis functions becomes asymptotic. Fig 8.1 shows the plot for the \( j=0, v=0 \) energy without the strong interaction. For each point, the energy value plotted is the best obtained by adjusting the non-variational parameters. The details of the wavefunction for each plotted point are recorded in Table 8.3.

The graphs in Figs 8.2 and 8.3 depict the real and imaginary parts of the energy for the case when the strong interaction is
Fig. 8.1. Graph of $j=0$, $v=0$ binding energy against number of basis functions for the case of no strong interaction.
<table>
<thead>
<tr>
<th>$n_b$</th>
<th>Energy (eV)</th>
<th>Channel $t_a$</th>
<th>$l_a$</th>
<th>$n_i$</th>
<th>$r_{min}$ (F)</th>
<th>$r_{max}$ (F)</th>
<th>$n_j$</th>
<th>$R_{min}$ (F)</th>
<th>$R_{max}$ (F)</th>
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Table 8.3. Wavefunction details for the points plotted in Fig. 8.1. $n_b$ is the number of basis functions.
introduced into the calculation. As before the abscissa is the number of basis functions. The details of the wavefunctions are given in Table 8.4. For this state, the final results are collected in Table 8.5. Also given there are the expectation values of various powers of all three inter-particle distances for one of the numerous trial functions used in the calculation.

SECTION 8.7 - RESULTS FOR EXCITED STATES

When the strong interaction is included in the calculation for \( j=0 \) state energies, with the threshold energy fixed at the value from Bohr's formula, negative values appear for the \( v=1 \) state as well. This indicates that the strong force might be producing a new bound state. The non-variational parameters are adjusted to find the lowest value for the energy. As usual, one configuration is first employed. The results are tabulated in Table 8.6. It is observed that the energy does not exhibit a minimum with respect to the size parameter \( R_{\text{max}} \) but always falls as this is increased. But it tends to a certain value as the parameter grows very large. On introducing other configurations, their effect is found to be negligible. This fact indicates that, far from being an excited-state energy for the \( \text{ppK} \) system, it is actually for the kaonic-hydrogen atom. In the next chapter, it is shown that the new eigenvalue gives the strong-interaction shift and width for the \( \text{is} \) state of kaonic hydrogen. The best value obtained here is \((\text{shift, width}) = (-400.4, 1074.7) \text{ eV}\).

In many generalized hydrogen molecular ions, the \( j=1, v=0 \)
Fig. 8.2. Graph of real part of $\nu=0$, $\nu=0$ energy against number of basis functions.
Fig. 8.3. Graph of $j=0$, $v=0$ width against number of basis functions.
<table>
<thead>
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<th>Energy (eV)</th>
<th>Channel</th>
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<th>$l_a$</th>
<th>$n_l$</th>
<th>$r_{min}$ (F)</th>
<th>$r_{max}$ (F)</th>
<th>$n_j$</th>
<th>$R_{min}$ (F)</th>
<th>$R_{max}$ (F)</th>
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<td>10</td>
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</tbody>
</table>

Table 8.4. Wavefunction details for the points plotted in Figs. 8.3 and 8.4. The negative part of the energy is the binding energy and the other part is the absorption width. Continued on next page.
<table>
<thead>
<tr>
<th>n_b</th>
<th>Energy (eV)</th>
<th>Channel 1 a</th>
<th>n_i</th>
<th>r_min (F)</th>
<th>r_max (F)</th>
<th>R_min (F)</th>
<th>R_max (F)</th>
</tr>
</thead>
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<td>3 0 0 10 20</td>
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<td>3 0 0 10 20</td>
<td>500</td>
<td>10 20 800</td>
</tr>
</tbody>
</table>

Table 8.4. Wavefunction details for the points plotted in Figs. 8.3 and 8.4. The negative part of the energy is the binding energy and the other part is the absorption width.
Electromagnetic binding energy = 491.3 eV
Total binding energy = 515.0 eV
Strong-interaction shift = -23.7 eV
Strong-absorption width = 1141.7 eV

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<td>6.50</td>
<td>2.87</td>
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<td>55.1</td>
<td>55.0</td>
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</table>

Expectation values for the several channels $a$. Fig. 7.1 shows which separation distance each operator pertains to. $\langle r_0 \rangle$ is in units of $a_0$ and $\langle r_a^2 \rangle$ in units of $a_0^2$ where $a_0$ is the kaonic-hydrogen Bohr radius.

Details of the wavefunction used to obtain the expectation values above. The imaginary part of the energy has already been converted to the width.

Table 8.5. Final results for the $j=0$, $v=0$ state.
Table 8.6. Dependence of the J=0, v=1 energy on the size parameters $R_{\text{min}}$ and $R_{\text{max}}$. The other parameters are fixed and are $r_{\text{min}} = 18F$, $r_{\text{max}} = 600F$, $n_i = 10$, $n_j = 1$, channel=1, and $(\alpha_a, \alpha_a) = (0.0)$. The imaginary part of the energy has been converted to the width.

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<th>Energy (eV)</th>
<th>$R_{\text{min}}$ (F)</th>
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</tbody>
</table>
level is bound; sometimes, the \( v=1 \) state is as well [115]. For this reason, this state is reported on next. Normally, a few experiments with the size parameters suffice to reveal the presence of a bound state. But no negative eigenvalues which could be interpreted as being for bound states of the ppK system appeared for either the case of the full potential or the case of the electromagnetic potential only. The conclusion is that the \( j=1, v=0 \) state is not bound in the ppK molecule. This important result is considered from another angle.

In the pp\( \mu \) system, the \( j=1, v=0 \) state is bound. The primary difference between this ion and the ppK ion from the point of view of the variational code is the value of the negatively-charged mass. Therefore a plot of the \( j=1, v=0 \) energy against the mass of the negative particle should show a meaningful dependence between the two quantities. The graph should have a positive slope and should intersect the energy axis at a mass value smaller than the kaon mass. To start with, the binding is assumed to be caused entirely by the Coulomb interactions, and the electromagnetic energy is examined first. Extra points for the plot are secured by employing some fictitious molecular ions. The masses of the negative particles in these ions are obtained from the kaon value by multiplying it by the fraction given as the second entry of data on line 1.

The resulting graph is presented in Fig 8.4. It conforms with expectation and proves conclusively that the ppk system has no \( j=1, v=0 \) excited state when the strong interaction is absent. As a matter of interest, it should be observed that the energy values used in the plot are all probably accurate to a few eV;
Fig. 8.4. Plot of $j=1, v=0$ energy against mass of negative particle in generalized hydrogen molecular ions. The energy for the ppK ion would correspond to the abscissa 493.78, and is out of the picture (to the right) on this scale.
Table 8.7. Dependence of the $J=1, v=0$ energy on the size parameters $R_{\text{min}}$ and $R_{\text{max}}$. The other parameters are fixed and are $r_{\text{min}} = 4.5F$, $r_{\text{max}} = 325F$, $n_i = 10$, $n_j=1$, channel=1, and $(\lambda_1, \lambda_a) = (0,1)$. There is no strong interaction. The table shows how the energy gives the ground-state value for kaonic hydrogen when the value of $R$ is very large. The energy is measured with respect to the uncorrected Bohr energy in kaonic hydrogen. The imaginary part of the energy has already been converted to the width.

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<td>1.8115</td>
<td>$10^7$</td>
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Table 8.8. Dependence of the $J=1, v=0$ energy on the size parameters $R_{\text{min}}$ and $R_{\text{max}}$. The other parameters are fixed and are $r_{\text{min}} = 18F$, $r_{\text{max}} = 600F$, $n_i = 10$, $n_j=1$, channel=1, and $(\lambda_1, \lambda_a) = (0,1)$. The real part of the energy is measured with respect to the uncorrected Bohr energy in kaonic hydrogen. The imaginary part of the energy has already been converted to the width.

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<td>(15058,461.0)</td>
<td>10</td>
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<tr>
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<td>1500</td>
<td>(-245.0,1068.8)</td>
<td>$10^6$</td>
<td>$1.5 \times 10^6$</td>
</tr>
<tr>
<td>10000</td>
<td>15000</td>
<td>(-398.7,1074.7)</td>
<td>$10^7$</td>
<td>$1.5 \times 10^7$</td>
</tr>
</tbody>
</table>
certainly, the value of the pp\(\mu\) energy is [115].

As an important exercise, the \(j=1, v=0\) energy is further investigated by adjustments to the size parameters. The results, are given in Table 8.7. Only one configuration of parameters has been used to express the wavefunction. The energy stays positive, but approaches a limit: from the very large values of the size parameter \(R_{\text{max}}\), it is once again clear that the interpretation of the results is the same as that given for the \(j=0, v=1\) energy. Again, the two-body limit of the three-body system, has naturally appeared. Thus, the energies in Tables 8.6 and 8.8 really pertain to kaonic hydrogen. Though not recorded here, it is observed that as \(R_{\text{max}}\) becomes larger, the energies of more vibrational states approach the limiting value. It is inferred that if \(R_{\text{max}}\) became infinite, the energies for all \(v\) states would stabilise at one value. This phenomenon is readily interpreted, and the topic is pursued further in the next chapter.

Next, the strong interaction is introduced. Now negative values do appear for the real parts of the results for the \(j=1, v=0\) state. They do not correspond to bound states of the ppK ion however, because, as the results in Table 8.8 show, the lowest values of energy are obtained when the size parameter \(R_{\text{max}}\) is very large. The same construction is put on the results as was done for the case of no strong interaction and the case of the \(j=0, v=1\) energy. The negative values appear when the strong interaction is on simply because the threshold energy used is the uncorrected Bohr value for all cases. The reason for initially using the uncorrected threshold energy in every case was that the 1s strong-interaction shift was not known beforehand. Making the
size parameter $R_{\text{max}}$ very large has provided this quantity; it is this very value which is quoted in an earlier part of this section. The tables show that when the strong interaction is off, choosing $R_{\text{max}}$ to be very large makes both the $j=0$, $v=1$ and the $j=1$, $v=0$ energies tend to the same limit. The same is true for the case when the strong force is present; both $j=0$, $v=1$ and $j=1$, $v=0$ energies tend to the same complex limit. The reason why the trial functions achieve the same form in this limit is given in the next chapter. In fact, all $j=0$ energies, including the one corresponding to $v=0$ should behave similarly. The same should hold true for all $j=1$ energies provided that in the channel 1, the combination $(1,\ell)$ should equal (0,1). These matters are discussed more fully in the next chapter.
SECTION 9.1 – THE THRESHOLD ENERGY

A brief note on the threshold energy is in order before the results given in Chapter 8 are analysed. The 1s energy in a hydrogen-like system is given basically by the Bohr formula (8.3). Corrections to it arise from the effects of relativity, vacuum polarization, the finite size of charge distributions and, in this case, the strong interaction. The last correction is the largest and adds to the basic value of -8614.0 eV a further -400.4 eV. The value used here for the shift is not in agreement with those in the literature [20-23]. However, it is plausible, and more importantly, since it proceeds naturally from this study, is the right one to use. The diversity of values in the literature for the strong-interaction shift and absorption rate, is illustrated by the compilation in ref. [20].

The corrected threshold energy is used only when the strong interaction is "on" in the ppK ion. To get the binding energy for the case when only electromagnetic forces operate, the uncorrected threshold energy is used. The values particular employed in his work have already been given in Chapter 8.
SECTION 9.2 - THE TWO-BODY LIMIT OF THE ppK ION

The reasons some of the energies given in Chapter 8 are to be identified as being for the 1s state of kaonic hydrogen are now given. It is useful to consult Tables 8.6 - 8.8 beforehand. The fact that only the coordinates of rearrangement channel 1 are involved in the description of the wavefunctions of these states is noted. From Fig 7.1 it is observed that in this channel, \( r_1 \) is the vector separating one proton and the kaon while \( R_1 \) is the displacement of the other proton from the centre of mass of these two.

From Tables 8.6 - 8.8, it is seen that, the energies monotonically decrease as the size parameter \( R_{\text{max}} \) is progressively increased. The definition of the coordinates shows that increasing \( R_{\text{max}} \) corresponds to effectively removing the odd proton from the vicinity of the other two particles. Thus, the greater \( R_{\text{max}} \) is, the closer the configuration of the particles approaches the situation where a kaonic hydrogen atom is feebly influenced by a distant proton. In that case, the energies should tend to those of kaonic hydrogen states.

Furthermore, the two body-system which remains after the odd proton is removed has angular momentum 0 for both \( j=0 \) and \( j=1 \). The radial part of the trial function is defined only by the Gaussian functions; it has no node and can only faithfully describe the 1s state and no other. So all \( N \) eigenvalues should tend to the same value as \( R_{\text{max}} \) goes to infinity. This is confirmed; as \( R_{\text{max}} \) is increased, more of the eigenvalues approach the limiting value. Since these particular energies are measured
with respect to the electromagnetic energy of the 1s state in
kaonic hydrogen, the limiting values should be zero for the case
of no strong interaction, and should be the kaonic hydrogen shift
and width for when this potential is included. This is why the
values from Table 8.8 are interpreted as the kaonic hydrogen 1s
strong-interaction effects.

SECTION 9.3- ANALYSIS OF ENERGY RESULTS

The single bound state of the ppK system has binding energy
515.0 eV and an electromagnetic contribution of 491.3 eV, so that
the strong-interaction shift is -23.7 eV. The absorption width is
1141.7 eV.

The electromagnetic energy of the j=0, ν=0 state is in
keeping with the results for other three-body ions [59,115] ;
thus the binding is tighter in this system than in the ppμ or ppπ
ions because this quantity goes up with mass of negative particle
in hydrogen molecular ions.

Because of the strong interaction, the binding of the ppK
ion is increased. This effect rather than the opposite is
produced peculiarly because of the strong potential selected for
use. Any potential constructed from the experimental data would
lead to the binding being relaxed.

The strong-interaction shift in this system is very much
smaller than the width, while in kaonic atoms, the ratio of the
one to the other is about a quarter [116]. Obviously, the greater
contrast here is a consequence of the fact that only the real part
of the 1s kaonic-hydrogen energy is involved in the definition of
the threshold energy, so that a good part of the absolute ppK
shift is neutralized by the the 1s shift. The width values from
the two-body and three-body systems are closer to one another than
the shift values. A comparison of the 1s width with the ppK width
shows that the second is slightly greater. The fact that the ppK
j=0, v=0 width is not too much greater than the kaonic-hydrogen
width is due to a conjunction of two factors. The strong
interaction falls off very rapidly with distance; however despite
the greater average separations of the particles in the molecule,
there are two protons for the kaon to interact with and the
combined effect compensates for the reduced two-body interactions.

The plot of the J=1, v=0 energy versus the mass of negative
particle in the exotic hydrogen molecular ion has shown the
absence of a bound state with these quantum numbers. Part of the
reason for this has to do with the threshold energy. As the mass
of the exotic particle increases, the threshold energy and the
absolute J=1, v=0 energies decrease. But the threshold energy
decreases faster than the absolute energy, and the difference
between these two becomes ever larger until it is positive and the
state is no longer bound. A plot of the threshold energies and
the absolute J=1, v=0 energies for the fictitious masses appearing
in Fig 8.4 is shown in Fig. 9.1 to demonstrate this. The mass
value corresponding to the intersection of the graphs shows at
what point generalized hydrogen molecular ions cease to have the
J=1, v=0 bound state.
Table 9.1. Comparative plot of electromagnetic threshold energy and absolute $j=1, v=0$ energy for fictitious hydrogen molecular ions. Kaon mass would be out of the picture.
In Chapter 7, the most important expectation values for the ppk system were listed, and sample values for them were reported in Table 8.5. During the calculation, it was found that though the energy of a particular state decreased each time the number of basis functions was increased, there was no similar consistent behaviour on the part of the expectation values. On the contrary, unsystematic fluctuations were observed from one trial function to another. For this reason, the accuracy of the expectation values in Table 8.5 is doubtful.

The fact that the wavefunctions are not reliable for the computation of expectation values, even though they yield accurate energies, proceeds from two factors. It has already been remarked that it is characteristic of the variational method to give energies suffering only from second-order error while the wavefunction is subject to first-order error. This is one source of difficulty. However, the more important reason is that the Gaussian trial function has a fast-decaying tail which cannot reproduce the more gentle fall-off of the actual wavefunction. As a result, expectation values of operators whose maximal values lie near the asymptotic regions are seriously affected. If the wavefunction is required for further work, it is more appropriate to use a different radial trial-function form, such as the exponential. Alternatively, the present wavefunctions could be improved by taking rather large size parameters, and using more basis functions to counteract the fact that such values are not
optimum. These questions, however, constitute another problem altogether; in this work the energy is the prime concern and the issue of wavefunction accuracy need not be pursued further.

SECTION 9.5 - GENERAL IMPLICATIONS

The way in which the three-body binding energies are measured promotes the importance of effects which are normally second- and higher-order. Thus the strong-interaction absorption width is twice the binding energy in the ppK ion. With respect to the absolute energy, the width is only about 12% in value; its relative magnitude is simply exaggerated by the circumstance that the binding energy is itself only a small fraction of the absolute energy. It is inferred from this that any effect which appears in the ppK ion but not in kaonic hydrogen might have a profound and disproportionate influence on the measurable energy because there is no term in the threshold energy which neutralizes some of its contribution in the ppK system in the same way that the 1s strong-interaction shift and the 1s Bohr energy have done to the corresponding quantities in the molecule. In other words, the absolute value of such an effect fully bears on the effective molecular binding energy. This fact has one very important consequence. The nuclear force between the two protons can no longer be assumed to change the binding energies only slightly.

This study has adhered to the past practice of ignoring the proton-proton nuclear force. In other exotic-particle hydrogen molecular ions, this omission has been motivated by the relatively
large size of the molecules, which has supported the idea that the force is negligible. The ppK system is much more compact however. A good guide to the relative sizes of the ppK system and the ordinary ppe system is provided by the Bohr radii of the corresponding species of hydrogen. The kaonic-hydrogen Bohr radius is about 633 times smaller and this is about how much smaller than the ppe ion the ppK ion is. Of course, this in itself does not guarantee that the proton-proton force is important; but the importance of proton-kaon strong-interaction effects strongly supports the suspicion that it is. While it is true that the proton-proton separation should be greater on average than the kaon-proton value, the difference should be small, to judge from the results for other three-body sytems [114] (no conclusion should be drawn from the obviously anomalous expectation values in Chapter 8).

Other corrections to the ppK energies - due to relativistic and vacuum-polarization effects - appear in kaonic hydrogen as well, and are partially neutralised when the threshold energy is subtracted from the absolute values. The relativistic effects are properly taken account of in the two-body case by the use of the Klein-Gordon equation instead of the Schroedinger equation. But the Klein-Gordon equation does not lend itself readily to many-body applications. Fortunately, the advantages of the Schroedinger equation need not be sacrificed for the sake of relativistic effects; The Breit-Pauli Hamiltonain [57] incorporates them within the framework of the Schröedinger formulation.
One of the original aims of this study was to deduce, by study of the ppK system, some properties of the ppp$^-$ and the pp$^-$ systems. Some generalizations are indeed possible. In these ions, the negative particle is heavier than in the ppK case. Therefore, the electromagnetic $j=0, \nu=0$ binding energy is higher. It also follows from Fig 8.4 that the $j=1, \nu=0$ level is unbound in both cases, unless the strong interaction should mediate otherwise.

The signs of the strong-interaction shifts should turn out to be opposite in the ppp$^-$ and pp$^-$ molecules. In the ppp$^-$ ion, the situation is akin to that in the ppK case; the binding is increased by the strong force. This effect is in keeping with the negative signs observed in the atomic shifts [19]. But as the shift is positive in sigma atoms [18,19], the binding of the pp$^-$ levels is loosened. The sizes of the shifts and widths in the two new ions should be larger than in the ppK case because of the greater magnitude of the shift and the width in the atomic systems.

In relation to the binding energy of certain shallow exotic-molecule levels, the $j=0, \nu=0$ strong-interaction shift of -23.7 eV in the ppK system is quite high. For example, the $j=1, \nu=1$ level in the dt$\mu$ molecule has a binding energy of only 0.659 eV [17]. The question arises whether the strong interaction could alter the status of molecular levels from being bound to being unbound or vice-versa. The reply is that this is unlikely. The shift for any bound excited state is certain to be an order of magnitude smaller than the value for the $j=0, \nu=0$ level, since the
very localised strong force is extremely sensitive to interparticle distances and falls off very fast with any expansion of the orbit. In subtracting the threshold energy from the absolute energies to get the binding energies, every strong-interaction shift is essentially being compared to that for the 1s level in the two-body system which the threshold energy is drawn from. Therefore, in every excited-state case, the shift should be more or less attenuated to very small magnitude by the subtraction process.

SECTION 9.6 - SUGGESTIONS FOR FUTURE WORK

Before all the forces in the system are properly taken into account, the ppK binding energy cannot be authoritatively given. Therefore, the first step in the improvement of the calculation is to introduce the proton-proton nuclear force and to improve the description of the proton-kaon strong interaction. As emphasized above, this is likely to affect the binding energy very significantly. In this connection, it should be remembered that the binding energies of other exotic-particle hydrogen molecular ions are known to an accuracy of fractions of eV. This degree of accuracy will have to be achieved before the value of the ppK total binding energy is accepted. The values quoted here are much less accurate; this is especially true for the full value which suffers from the uncertainty in the form of the proton-kaon strong potential in addition to the neglect of the proton-proton force.

Lesser improvements ought to be effected by the
relativistic and the vacuum-polarization corrections, but these effects should be studied for the sake of completeness and of confirming that they are indeed unimportant.

An issue of formal importance arises from the fact that by introducing the non-Hermitian strong interaction, one of the premises of Theorem 1 in Chapter 6 has been violated. No obvious method of gauging the influence on the results of this slight departure from rigour has presented itself. The reason for assuming that it is small is that the Hamiltonian is "only slightly" non-Hermitian as a result of the appearance of the imaginary part of the strong potential. Nevertheless, this issue also demands rigorous treatment.

SECTION 9.7 - CONCLUSIONS

This study of the ppK ion has realized some of the objectives stated at the outset, but not all.

The domain of the Born-Oppenheimer approximation has been found to be no wider than might be expected. It is clear from the qualitative, though still-valid, considerations of Chapter 5 that it is of little use in the study of the ppK, ppp⁻ and ppΣ⁻ ions.

The ppK system has been found to exist in only the ground state, but the effort to give the energy of this state with the degree of accuracy achieved in studies of similar molecules has been only partially successful, frustrated by the long-standing problem of the kaon-proton interaction. This stresses the urgency with which the issue of understanding the
kaon-proton force should be treated. Despite these difficulties, important qualitative conclusions have been drawn, some with immediate generalisation to the ppp and ppE systems. A special one is the realization that the proton-proton force cannot be overlooked in compact molecules. Indeed, due to the fact that most of the electromagnetic contribution to the energy is lost when the threshold reference level is subtracted, the effects on the system of any perturbations which appear in the molecular case but not in the two-body case are enhanced.

No evidence has been uncovered to show that the ppK ion in any way influences measurements on kaonic hydrogen. Therefore little illumination has been shed on the kaonic hydrogen problem; nevertheless, the importance of strong-interaction effects, particularly the width, in the ppK system, has been demonstrated. Thus this ion affords one more system in which the elementary interaction between the kaon and the proton might be studied experimentally.

The absence of excited states in the ppK molecule has meant that some work done on dipole transition rates was in vain; in retrospect it can be seen that the unreliability of the wavefunctions - shown by the poor expectation values - would have complicated the job of predicting accurate X-ray intensities.

This study of the ppK system is by no means complete, but it has yielded useful information. It is hoped that some of the suggestions for improvement of the calculation will be taken up, and that when experiments are performed on the ion, this work will provide useful guidance.
APPENDIX A - TRANSFORMATION OF THE HAMILTONIAN FROM LABORATORY TO INTERNAL COORDINATES

In laboratory coordinates, the three-body system Hamiltonian is given by expression (5.1). Its form in terms of the internal coordinates is given by expression (5.6). In this appendix, the transformation from the first form to the second is given in detail.

In terms of the laboratory coordinates \( x_1, x_2 \) and \( x_3 \), the generalised internal coordinates are [2-8]

\[
X = \frac{m_1 x_1 + m_2 x_2 + m_3 x_3}{m_1 + m_2 + m_3}, \quad (A1)
\]

\[
r = x_2 - x_1, \quad (A2)
\]

and

\[
R = x_3 - (\beta_1 x_1 + \beta_2 x_2)/(\beta_1 + \beta_2), \quad (A3)
\]

where \( \beta_1 \) and \( \beta_2 \) are constants. As was mentioned in Chapter 7, the definitions of \( r \) and \( R \) given above represent just one set out of a possible three, but here, for simplicity, the subscripts which distinguish this choice from the other two are omitted. To illustrate the transformation, only one choice need be dealt with, of course, since the other two transformations are achieved by
exactly the same method.

The generalised transformation to be given here has been used extensively by Ponomarev and Vinitskii [4,5,22,45-47,50,51] in their work on mesonic atoms. Slightly different forms have been given by Hunter et al [6], by Fröman and Kinsey [8] and by Pack and Hirschfelder [97,98]; the last authors derive a separation of coordinates for an arbitrary diatomic system.

In terms of the new coordinates, the laboratory ones are

\[
x_1 = \frac{M(\beta_1 + \beta_2)X - [m_2(\beta_1 + \beta_2) + m_3 \beta_2]R - m_3(\beta_1 + \beta_2)r}{M(\beta_1 + \beta_2)}, \quad (A4)
\]

\[
x_2 = \frac{M(\beta_1 + \beta_2)X - [m_1(\beta_1 + \beta_2) + m_3 \beta_1]R - m_3(\beta_1 + \beta_2)r}{M(\beta_1 + \beta_2)}, \quad (A5)
\]

and

\[
x_3 = \frac{M(\beta_1 + \beta_2)X + (m_1 \beta_2 - m_2 \beta_1)R + (m_1 + m_2)(\beta_1 + \beta_2)r}{M(\beta_1 + \beta_2)}, \quad (A6)
\]

where \( M \) is the total mass.

The squares of the momentum operators are, of course, given by

\[
p_i^2 = -\hbar^2 \nabla_i^2 x_i, \quad (i = 1, 2, 3), \quad (A7)
\]

with the Laplacians given by

\[
\nabla_i^2 x_i = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} = \frac{\partial^2}{\partial x_i^2}, \quad (A8)
\]
where

\[ \mathbf{x}_i = \mathbf{x}_i(X,R,r). \quad (A9) \]

Using the differentiation chain rule on (A9) yields

\[
\begin{align*}
\frac{\partial^2}{\partial x_i^2} & = c_1^{(i)} \frac{\partial^2}{\partial x^2} + c_2^{(i)} \frac{\partial^2}{\partial R^2} + c_3^{(i)} \frac{\partial^2}{\partial r^2} \\
& + c_1^{(i)} c_2^{(i)} \left( \frac{\partial^2}{\partial R \partial X} + \frac{\partial^2}{\partial X \partial R} \right) + c_1^{(i)} c_3^{(i)} \left( \frac{\partial^2}{\partial r \partial X} + \frac{\partial^2}{\partial X \partial r} \right) \\
& + c_2^{(i)} c_3^{(i)} \left( \frac{\partial^2}{\partial R \partial r} + \frac{\partial^2}{\partial r \partial R} \right), \quad (A10)
\end{align*}
\]

where

\[
\begin{align*}
c_1^{(i)} & = \frac{\partial X}{\partial x_i}, \quad (A11) \\
c_2^{(i)} & = \frac{\partial R}{\partial x_i}, \quad (A12)
\end{align*}
\]

and

\[
\begin{align*}
c_3^{(i)} & = \frac{\partial r}{\partial x_i}. \quad (A13)
\end{align*}
\]

In (A10)-(A13), the labels 1,2 and 3 have been arbitrarily assigned to the coordinates X, R and r respectively for convenience.

Apart from the constant \(-\hbar^2\), the kinetic-energy part of the Hamiltonian is

\[
\begin{align*}
\sum_i \frac{\mathbf{v}_i^2}{2m_i} & = \left( \sum_i c_1^{(i)} \right)^2 \frac{\partial^2}{\partial x_i^2} + \left( \sum_i c_2^{(i)} \right)^2 \frac{\partial^2}{\partial R_i^2} \\
& + \left( \sum_i c_3^{(i)} \right)^2 \frac{\partial^2}{\partial r_i^2} + \left( \sum_i c_1^{(i)} c_2^{(i)} \right) \frac{\partial^2}{\partial X \partial R} + \frac{\partial^2}{\partial R \partial X}
\end{align*}
\]
\[
\begin{align*}
+ ( \sum_{i} c_{1}^{(1)} c_{3}^{(1)}/2m_{1}) (\partial^{2}/\partial X \partial r + \partial^{2}/\partial r \partial X) \\
+ ( \sum_{i} c_{2}^{(1)} c_{2}^{(1)}/2m_{1}) (\partial^{2}/\partial R \partial r + \partial^{2}/\partial r \partial R),
\end{align*}
\]

(A14)

with all the summations running from 1 to 3.

From the relations (A4)-(A6), the \(c's\) are obtained:

\[
\begin{align*}
c_{1}^{(1)} &= m_{1}/M, \quad c_{1}^{(2)} = m_{2}/M, \quad \text{and} \quad c_{1}^{(3)} = m_{3}/M; \\
c_{2}^{(1)} &= -1, \quad c_{2}^{(2)} = 1, \quad \text{and} \quad c_{2}^{(3)} = 0;
\end{align*}
\]

(A15)

and

\[
\begin{align*}
c_{3}^{(1)} &= -\beta_{1}/(\beta_{1} + \beta_{2}), \quad c_{3}^{(2)} = -\beta_{2}/(\beta_{1} + \beta_{2}), \quad \text{and} \quad c_{3}^{(3)} = 1.
\end{align*}
\]

(A16)

When these are inserted into (A14), the result is

\[
\begin{align*}
\sum_{i} \frac{\nabla^{2} x_{i}}{2m_{1}} &= (1/2M)\partial^{2}/\partial X^{2} + (1/2)(1/m_{1} + 1/m_{2})\partial^{2}/\partial R^{2} \\
&\quad + (1/2)[\beta_{1}^{2}/m_{1}(\beta_{1} + \beta_{2})^{2} + \beta_{2}^{2}/m_{2}(\beta_{1} + \beta_{2})^{2} + 1/m_{3}]\partial^{2}/\partial r^{2} \\
&\quad + (1/2)[\beta_{1}/m_{1}(\beta_{1} + \beta_{2}) - \beta_{2}/m_{2}(\beta_{1} + \beta_{2})] (\partial/\partial R \partial/\partial r + \partial/\partial r \partial/\partial R). \quad \text{(A18)}
\end{align*}
\]

In (A18), the coefficients of the two sets of cross-derivatives involving \(\partial/\partial X\) have vanished, which is expected if the motion of the centre of mass is to be decoupled from the internal motion. To put the coefficient of the remaining cross-derivatives in a more concise form, the quantity

\[1/M = 1/(m_{1} + m_{1})\]

is first factored from it. Thus,

\[
C = \left(\frac{m_{1} + m_{2}^{2}}{m_{1} m_{2}}\right) \left(\frac{m_{1} m_{2}^{2}}{m_{1}^{2} + m_{2}^{2}}\right) \left(\frac{m_{2} \beta_{1} - m_{1} \beta_{2}}{m_{1} m_{2}(\beta_{1} + \beta_{2})}\right),
\]

(A18)
where $C$ denotes this coefficient. Now

$$m_2\beta_1 - m_1\beta_2 = m_2\beta_1 - m_1\beta_2 - m_1\beta_1 - m_1\beta_1$$

$$= (m_2 - m_1)\beta_1 - m_1 (\beta_2 - \beta_1)$$

$$= m_2\beta_1 - m_1\beta_2 - m_2\beta_2 + m_2\beta_2$$

$$= (m_2 - m_1)\beta_2 - m_2 (\beta_2 - \beta_1)$$

$$= (1/2)[(m_2 - m_1)(\beta_2 - \beta_1) - (m_2 + m_1)(\beta_2 - \beta_1)].$$

Hence

$$C = (1/2M_a) \frac{m_2 - m_1}{m_2 + m_1} - \frac{\beta_1 - \beta_2}{\beta_2 + \beta_1}$$

$$= a/4M_a,$$

where $a$ is the quantity in the brackets in (A23).

To simplify the coefficient of $\beta^2/\partial r^2$, the quantity $1/(m_1 + m_2)$ is added and subtracted inside the brackets to give

$$C' = (1/2)[\frac{m_2\beta_1^2 + m_1\beta_2^2}{m_1 m_2 (\beta_1 + \beta_2)^2} - \frac{1}{m_1 + m_2}] + (1/2)[\frac{1}{m_3} + \frac{1}{m_1 + m_2}].$$

Factoring $1/m_a$ from the first term and dividing it by the lowest common multiple yields

$$C' = (1/2M_a) \frac{(m_2\beta_1 - m_1\beta_2)^2}{(m_1 + m_2)^2 (\beta_1 + \beta_2)^2} + 1/2m_a,$$

where
\( \frac{1}{m_a} = \frac{1}{m_3} + \frac{1}{(m_1 + m_2)}. \) \hspace{1cm} (A27)

Comparing this with (A19) and (A23) shows that it may be written as

\[ C' = \left(\frac{1}{2M_a}\right) \left(\frac{a^2}{4}\right) + \frac{1}{2m_a}. \] \hspace{1cm} (A28)

Using (A23) and (A28) in (A18) after multiplying by \(-\hbar^2\) gives finally the transformed Hamiltonian quoted in Chapter 5:

\[ H = \left(-\hbar^2/2M\right) \nabla^2 - \left(-\hbar^2/2M_a\right) \left[ \nabla_R^2 + \left(\frac{a}{2}\right) \left( \nabla_R \nabla_R + \nabla_R \nabla_R \right) + \frac{a^2}{4} \nabla_R^2 \right] \]
\[ - \left(-\hbar^2/2m_a\right) \nabla_R^2 + V(r, R). \] \hspace{1cm} (A30)
APPENDIX B - DETAILED DERIVATION OF THE INTERACTION MATRIX ELEMENT

This appendix illustrates the methods by which the formulas for the matrix elements given in Chapter 7 are obtained. The interaction matrix element is derived, and since its derivation involves the most effort, it is well suited to demonstrate these techniques.

The trial function $\psi$ used in this modification of the variational technique is an explicit function of all three sets of rearrangement Jacobi coordinates of the three-body system. As explained in Chapter 7, the Jacobi coordinates are not independent of each other, but are only different expressions of the same reality. For formal purposes, when the matrix elements are set up, one single choice of the rearrangement coordinates is used for the volume element. But for the practical integration, the most convenient of the coordinates appearing in the matrix elements are used for the integration variables. In the case of many interactions, the potential is a function only of inter-particle distances and the form of $V$ is particularly simple and convenient in the rearrangement channel $c$ in which the interparticle distance is given as $|r_c|$. To illustrate - the coordinates in which the Coulomb interaction between particles 1 and 3 is most simply given are those of channel 2, and they would be used as the integration
variable for the matrix element of this term of the potential. Thus, the integration is over the coordinates of that channel $c$.

It should be noted that the overlap and kinetic matrix elements both contain at most only two sets of coordinates and are consequently structurally simpler. Once this appendix has been understood, it should be an easy exercise to confirm all the formulas for the matrix elements given in Chapter 7.

For any operator $V$, the matrix element between basis functions $\phi_k(a)$ and $\phi_{k'}(b)$ is

$$M = \langle \phi_k(a) | V(c) | \phi_{k'}(b) \rangle,$$

(B1)

where generally, three sets of Jacobi coordinates $a$, $b$ and $c$ appear. The basis functions are [17,83-85]

$$\phi_k(a) = N \exp(-\frac{r^2}{2} - \frac{R^2}{2}) [Y^l(r_a) \otimes Y^l(R_a)]_{JM},$$

(B2)

and

$$\phi_{k'}(b) = N \exp(-\frac{r'^2}{2} - \frac{R'^2}{2}) [Y^l(r_b) \otimes Y^l(R_b)]_{JM}.$$  

(B3)

Both basis functions have to be transformed to the coordinates $c$ of the interaction $V(r_c)$, which serve as the variables of integration. For this purpose, the Raynal transformation [112]

$$r'^l R'^l [Y^l(r') \otimes Y_l^l(R')]_{JM} =$$
is used. The transformation coefficient is [109]

\[
\sum_{1L'T} <1'1J'|1LTJ> r'' \rightarrow r r'' r^{1' + l' + l'' - T} R^T [Y_{1'}(r) \otimes Y_{1''}(R)]_{JM} \tag{B4}
\]

\[
\langle 1'1' \mid 1LTJ \rangle_{r'' \rightarrow r} = (21' + 1)(2L' + 1)
\]

\[
\times \sum_{\alpha=0} \gamma'^{1'-\alpha} \gamma^{1'-l'-r+\alpha} \sum_{\delta=0} \delta^{1'-l'-r+\alpha} \left[ \begin{array}{c} 21' \\ 2L' \end{array} \right] \left[ \begin{array}{c} 21' \\ 2(1'-\alpha) \end{array} \right]^{1/2}
\]

\[
\times (1'-\alpha 0_{l'-r+\alpha} 0_{1'-r+\alpha} 0_{L'}) \left\{ \alpha^{1'-\alpha} \begin{array}{ccc} 1' \end{array} \right\} \left\{ l' \begin{array}{ccc} 1' \end{array} \right\} \left\{ \begin{array}{ccc} 1' \end{array} \right\} . \tag{B5}
\]

In terms of the new vectors, the old vectors are

\[
r' = \gamma r + \delta R \tag{B6}
\]

and

\[
R' = \gamma r' + \delta' R. \tag{B7}
\]

The limits in (B4) are

\[
0 \leq \tau \leq 1' + l', \tag{B8}
\]

\[
0 \leq 1 \leq 1' + l', \tag{B9}
\]

and

\[
0 \leq L \leq 1' + l'. \tag{B10}
\]

With

\[
]^{*} \right]
\]
\[
\Sigma \langle 1_{a}L_{j} | 1_{c}L_{j}, \tau > \rightarrow 1_{a}L_{j} \rightarrow 1_{c}L_{j} \rightarrow Y^\tau [Y^\tau (r_a) \otimes Y^\tau (r_b)]^* \quad (B11)
\]

and

\[
r^b R^L_a [Y^\tau (r_a) \otimes Y^\tau (r_b)]_{JM} =
\]

\[
\Sigma \langle 1_{b}L_{j} | 1_{c}L_{j}, \tau > \rightarrow 1_{b}L_{j} \rightarrow 1_{c}L_{j} \rightarrow Y^\tau [Y^\tau (r_a) \otimes Y^\tau (r_b)]^* \quad (B12)
\]

the matrix element becomes

\[
M = N N \Sigma \langle 1_{a}L_{j} | 1_{c}L_{j}, \tau > \rightarrow 1_{b}L_{j} \rightarrow 1_{c}L_{j} \rightarrow Y^\tau [Y^\tau (r_a) \otimes Y^\tau (r_b)]^* \quad (B13)
\]

The exponent is

\[
\nu (r^2 + \lambda R^2) + \nu (r^2 + \lambda R^2) =
\]

\[
\nu (\gamma r^2 + \delta R^2) + \nu (\gamma' r^2 + \delta' R^2)
\]

\[
+ \nu (\gamma r^2 + \delta R^2) + \nu (\gamma' r^2 + \delta' R^2)
\]

\[
= \eta r^2 + \zeta R^2 + 2 \xi r \cdot R
\]

where
\[ \eta = \nu \gamma^2 + \lambda \gamma' + \nu \gamma' + \lambda \gamma'^2 \]  
\[ \zeta = \nu \delta^2 + \lambda \delta' + \nu \delta + \lambda \delta'^2 \]  

and

\[ \xi = \nu \gamma \delta + \lambda \gamma' \delta' + \nu \gamma \delta' + \lambda \gamma' \delta' \]  

A modification of the Rayleigh expansion for the plane wave gives [85]

\[ \exp(-2\xi r \cdot R) = \sum_{\lambda=0}^{\infty} 4\pi\lambda \mathcal{J}_\lambda(2\xi r R) Y_\lambda(r) Y_{\lambda}(R) \]  

where \( \mathcal{J}_\lambda \) is the spherical Bessel function of imaginary argument of order \( \lambda \), related to the ordinary spherical Bessel function by

\[ \mathcal{J}_\lambda(x) = i^{-\lambda} j_\lambda(ix). \]

Using this formula, the matrix element becomes

\[ M = \int \sum_{\lambda} 4\pi\lambda \mathcal{J}_\lambda(2\xi r R) Y_\lambda(r) Y_{\lambda}(R) \]

where

\[ I_A = \int \int [Y_\lambda(r) Y_{\lambda}(R)]^* \int [Y_\lambda(r) Y_{\lambda}(R)] \]  

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To simplify the integrand of (B21), the relation [85]

\[
[Y_{\lambda}(r_c) \delta \hat{Y}_{\lambda}^*(R_c)]_{\lambda \mu} = (-1)^{\lambda \mu} \delta_\lambda^\mu W(K_{\lambda} \delta \Lambda_{\lambda}^\Lambda)/4\pi h
\]

is used. Using the orthonormality of the spherical harmonics, it follows that

\[
I_A = (-1)^J \sum_{\lambda' \Lambda' \lambda} \delta_\lambda^\lambda W(K_{\lambda} \hat{Y}_{\lambda} \delta_{\Lambda' \Lambda}^\Lambda)/4\pi h
\]

\[
= (-1)^J \sum_{\lambda' \Lambda' \lambda} \delta_\lambda^\lambda W(1 \hat{Y}_{\lambda} \delta_{\Lambda' \Lambda}^\Lambda)/4\pi h \cdot (B23)
\]

The radial integral is

\[
I_R = \int dr dR r^a b^b c^c \hat{Y}_{\lambda}(r_c) \delta \hat{Y}_{\lambda}^*(R_c)
\]

\[
\times \exp(-\eta r^2 -\xi R^2) \sum_{\lambda \Lambda \lambda' \Lambda'} (2\xi r R_c).
\]

Provided that \(m\) is a positive integer, the integration over \(R_c\) can be performed by means of the formula [113]
\[
\int dR_c R_c^{2m+\lambda} \exp(-\zeta R_c^2) j_{\lambda}^2(2\zeta r_c R_c) = \\
\sqrt{\pi} m! \xi^\lambda \exp(\xi^2 r_c^2/\zeta) L_m^{\lambda+1/2}(-\xi^2 r_c^2/\zeta),
\]

(B26)

where \( L_m^{\lambda+1/2} \) is the associated Laguerre polynomial.

To show that \( m \) is a positive integer, conditions arising from the Clebsch-Gordan coefficients are used. All the Clebsch-Gordan coefficients which have appeared have vanishing magnetic quantum numbers. For such coefficients to be nonvanishing, the sum of non-zero arguments must be even, and the triangle inequality must be satisfied. Thus from the Clebsh-Gordan coefficients, including those in the Raynal-transformation coefficient, come the conditions

\[
1 + L_a - \tau + 1_c = \text{even}, \quad (B27)
\]

\[
\tau + L_c = \text{even}, \quad (B28)
\]

\[
1_b + L_b - \tau' + 1_c' = \text{even}, \quad (B29)
\]

\[
\tau' + L_c' = \text{even}, \quad (B30)
\]

\[
1_c + 1_c' + \lambda = \text{even} \quad (B31)
\]

and

\[
L_c + L_c' + \lambda = \text{even} . \quad (B32)
\]

Adding (B28) and (B30) gives
\[ \tau + \tau' + L_c + L'_c = \text{even}. \]  
\hspace{1cm} \text{(B33)}

Subtracting (B32) from (B33) gives

\[ \tau + \tau' - \lambda = \text{even} = 2m. \]  
\hspace{1cm} \text{(B34)}

Three of the triangle inequalities are

\[ 2\alpha - \tau \leq L_c \leq \tau, \]  
\hspace{1cm} \text{(B35)}

\[ 2\alpha' - \tau' \leq L'_c \leq \tau'. \]  
\hspace{1cm} \text{(B36)}

and

\[ |L_c - L'_c| \leq \lambda \leq L_c + L'_c. \]  
\hspace{1cm} \text{(B37)}

From (B35) and (B36) is deduced

\[ \tau + \tau' \geq L_c + L'_c, \]  
\hspace{1cm} \text{(B38)}

whence, since \( L \) and \( L' \) are positive integers,

\[ \tau + \tau' \geq 0. \]  
\hspace{1cm} \text{(B39)}

Using the fact from (B37) that \( \lambda \leq L_c + L'_c \), and subtracting \( \lambda \) from both sides of (B39) finally gives that

\[ \tau + \tau' - \lambda \geq 0. \]
Thus the radial integral over $R_c$ is given by (B26).

Unless the exact form of $V(r)$ is known, the radial integral cannot be completed. Nevertheless, the matrix element can be put in a form which makes this last task trivial. For this, the series form of the associated Laguerre polynomial [113]

$$I_m^{\lambda+1/2}(\xi \frac{r^2}{\zeta}) = (2m+2\lambda+1)!! \sum_{k=0}^{m} \left( \begin{array}{c} m \\ k \end{array} \right) \left( \frac{2\xi^2 r^2}{\zeta} \right)^k / (2k+2\lambda+1)!!$$  \hspace{1cm} (B40)

is needed. When it is inserted in the expression, the matrix element becomes

$$\langle \phi_k(a)|V(r_c)|\phi_{k'}(b)\rangle =$$

\begin{align*}
&\frac{\sqrt{\pi}}{4} (-1)^M N \sum_{a,b} \sum_{l} \langle l L J | 1' L' J' \rangle \langle 1 L J | c \rightarrow c \rangle \langle 1' L' J' | b \rightarrow c \rangle \\
&\times \xi^\lambda (2m+2\lambda+1)!! \sum_{c} \left( \begin{array}{c} m \\ k \end{array} \right) \left( \frac{2\xi^2 r^2}{\zeta} \right)^k U(r_c) / (2m+2\lambda+1)!! \\
&\equiv \frac{\xi^\lambda (2m+2\lambda+1)!!}{2^{m+\lambda+3/2} \zeta} \sum_{k=0}^{m} \left( \begin{array}{c} m \\ k \end{array} \right) \left( \frac{2\xi^2 r^2}{\zeta} \right)^k U(r_c) / (2m+2\lambda+1)!! .
\end{align*}

where

$$U(r_c) = \int dr_c r_c^a a^b b^c \exp(-\eta \xi^2 r_c^2) V(r_c^2).$$  \hspace{1cm} (B42)

If (B27), (B29) and (B31) are added together, the result is

$$1 + \lambda + l + 1 + l' - T - T' + 2k + 2 + \lambda = \text{even.}$$  \hspace{1cm} (B43)

Hence, the power of $r_c$ is $2n$, where
\[ n = \left( \frac{1}{a_a} + \frac{1}{a_b} + \frac{1}{L_b} - \frac{1}{\tau'} + 2k + 2 + \lambda \right)/2. \]  \hspace{1cm} \text{(B44)}

For functions \( V(r_c) \) in polynomial, inverse-power or Gaussian form, \( U(r_c) \) is given from the formulas [113]

\[ \int_0^\infty d r_c r_c^{2S+1}\exp(-pr_c^2) = \frac{s!}{2p^{S+1}}, \text{ for } p > 0 \]  \hspace{1cm} \text{(B45)}

and

\[ \int_0^\infty d r_c r_c^{2S}\exp(-pr_c^2) = \frac{(2s-1)!}{2(2p)^S} \left( \frac{\pi}{p} \right)^{1/2}, \text{ for } p > 0. \]  \hspace{1cm} \text{(B46)}

Whether \( p \) is positive or not obviously depends on \( \eta \xi - \xi^2 \).

From the definitions of \( \eta \xi \) and \( \xi \), this quantity is

\[ \eta \xi - \xi^2 = (\nu \gamma^2 + \lambda \gamma'^2 + \nu \gamma^2 + \lambda \gamma'^2) \left( \nu \delta^2 + \lambda \delta'^2 + \nu \delta^2 + \lambda \delta'^2 \right) \]
\[ - (\nu \gamma \delta + \lambda \gamma' \delta' + \nu \gamma \delta + \lambda \gamma' \delta')^2. \]  \hspace{1cm} \text{(B47)}

Some algebra recasts this quantity into the form

\[ \eta \xi - \xi^2 = \nu \lambda \left( \gamma \delta' - \gamma' \delta \right)^2 + \nu \nu \left( \gamma \delta' - \gamma' \delta \right)^2 \]
\[ + \nu \lambda \left( \gamma' \delta' - \gamma' \delta \right)^2 + \nu \lambda \left( \gamma' \delta' - \gamma' \delta \right)^2 \]
\[ + \lambda \lambda \left( \gamma \delta' - \gamma' \delta \right)^2 + \nu \lambda \left( \gamma \delta' - \gamma' \delta \right)^2. \]  \hspace{1cm} \text{(B48)}

Therefore \( p \) is either zero or positive. The first, third, fourth and last terms never vanish unless the size parameters do. In a normal calculation, all the \( \nu \)'s and \( \lambda \)'s are finite, and so the quantity on the left-hand side is never zero.
APPENDIX C - THE X-RAY DIPOLE TRANSITION MATRIX ELEMENT

SECTION C1 - INTRODUCTION

In this appendix, the expression for the matrix element for X-ray dipole transitions is given. It had been prepared in anticipation of finding bound excited states in the ppK ion and will find use in other three-body systems to which the Gaussian-expansion method might be applied.

The X-ray dipole matrix element between initial kaonic state \( \psi_i \) and final state \( \psi_f \) is

\[
M_t = \langle \psi_f | D | \psi_i \rangle, \tag{C1}
\]

where \( D \) is the dipole operator given by

\[
D = q_1 \mathbf{x}_1 + q_2 \mathbf{x}_2 + q_3 \mathbf{x}_3. \tag{C2}
\]

In (C2), \( q_k \) is the charge of the \( k \)-th particle. Since the wavefunctions are given by

\[
\psi_{iM_i} = \sum_k C_k \phi^{(k)}_{iM_i}, \tag{C3}
\]
and

\[ \Psi_{f f}^{M} = \sum_{1} c_{1} \phi^{(1)}_{f f} \]  

(C4)

terms in the expression for the matrix element are of the form

\[ M = <\phi_{j f}^{M}(a)|D(a)|\phi_{i i}^{M}(b)> . \]  

(C5)

Obviously, before (C5) can be used, the form of D in the Jacobi coordinates must be found.

SECTION C2 - THE DIPOLE OPERATOR IN JACOBI COORDINATES

In chapter 7, the coordinates \( x_1, x_2 \) and \( x_3 \) were given in Jacobi coordinates. Using the expressions in (C3) leads, after re-arranging, to the following expressions for D in each of the channels:

\[ D = (q_1 + q_2 + q_3)X + [(m_2 + m_3)q_1 - m_1 (q_2 + q_3)]R_1 / M \]
\[ + (m_2 q_3 - m_3 q_2) r_1 / (m_2 + m_3) = D_1 , \]  

(channel 1)  

(C6)

\[ = (q_1 + q_2 + q_3)X + [(m_1 + m_3)q_2 - m_2 (q_1 + q_3)]R_2 / M \]
\[ + (m_1 q_3 - m_3 q_1) r_2 / (m_1 + m_3) = D_2 , \]  

(channel 2)  

(C7)

\[ = (q_1 + q_2 + q_3)X + [(m_1 + m_2)q_3 - m_3 (q_1 + q_2)]R_3 / M \]
\[ + (m_2 q_1 - m_1 q_2) r_3 / (m_1 + m_2) = D_3 . \]  

(channel 3)  

(C8)
The effective operator in (C6), (C7) and (C8) excludes the first term because the wavefunctions on which D operates are not functions of X, and moreover are orthogonal. The vector parts of the effective operators can be expressed in terms of the coordinates of the problem by using the relation between vectors and spherical harmonics of order 1 [110]:

\[ Y_{1m}(\hat{r}) = \sqrt{\frac{3}{4\pi}} \frac{1}{r} \left\{ \begin{array}{c}
-(x+iy)/\sqrt{2} , \quad m=1 \\
z , \quad m=0, \\
(x+iy)/\sqrt{2} , \quad m=-1
\end{array} \right. \]  \hspace{1cm} (C9)

where \( \hat{r} \) is the direction of the vector \( r = (x,y,z) \). Thus

\[ x = \sqrt{\frac{2\pi}{3}} r \left[ Y_{1,-1}(\hat{r}) - Y_{11}(\hat{r}) \right], \]  \hspace{1cm} (C10)

\[ y = i\sqrt{\frac{2\pi}{3}} r \left[ Y_{1,-1}(\hat{r}) + Y_{11}(\hat{r}) \right], \]  \hspace{1cm} (C11)

and

\[ z = \sqrt{\frac{4\pi}{3}} r Y_{10}(\hat{r}). \]  \hspace{1cm} (C12)

If the effective dipole operator is written as

\[ D_j = d_j r_j + D_j R_j, \]  \hspace{1cm} (C13)

where \( d_j \) and \( D_j \) are given in (C6) - (C8), then in the spherical basis,

\[ D_j = x \sqrt{\frac{2\pi}{3}} \left( d_j r_j [Y_{1,-1}(\hat{r}) - Y_{11}(\hat{r})] + D_j R_j [Y_{1,-1}(\hat{R}) + Y_{11}(\hat{R})] \right) \]
where \( \hat{x} \), \( \hat{y} \) and \( \hat{z} \) are the unit vectors of the laboratory coordinate system.

Any term in (C14) has a form proportional to either \( rY_{1m}(\hat{r}) \) or \( RY_{1m}(\hat{R}) \). Therefore, to specify the transition probability, it is enough to give the matrix elements of these two operators. Only two sets of Jacobi coordinates need be involved in the expression, since \( D \) can always be chosen to be in the coordinates of one of the basis functions.

SECTION C3 - THE MATRIX ELEMENT OF \( rY_{1m}(\hat{r}) \)

For the basis functions \( \phi_k(a)_{JM} \) and \( \phi_k'(b)_{J'M'} \), the matrix element of the operator \( rY_{1m}(\hat{r}) \) is

\[
M = \int dr \, dR \, r^a \, a \, \exp(-\nu \, r^2 - \lambda \, R^2) [Y_{1m}(\hat{r}) \otimes Y_{1m}(\hat{R})]^* \times \left( \sum_{l, l'} \frac{\hat{r}^a \hat{R}^b}{a \, a \, a \, a} \right) \times \exp(-\nu \, r^2 - \lambda \, R^2) [Y_{1m}(\hat{r}) \otimes Y_{1m}(\hat{R})]_{j'M'} \, , \]  

(C15)

after the Raynal transformation has been used on the basis function \( \phi_k'(b) \).

The exponent in (C15) is

\[
-\nu \, r^2 - \lambda \, R^2 - \nu (\gamma \, r + \delta \, R)^2 - \lambda (\gamma' \, r + \delta' \, R)^2
\]
\[ = \eta r_a^2 - \zeta R_a^2 - 2\xi r_a \cdot R_a, \quad (C16) \]

where

\[ \eta = \nu_a + \nu_b \gamma_{ba}^2 + \lambda_b \gamma_{ba}, \quad (C17) \]
\[ \zeta = \lambda_a + \nu_b \delta_{ba}^2 + \lambda_b \delta_{ba}, \quad (C18) \]

and

\[ \xi = \nu \gamma_{ba} \delta_{ba} + \lambda \gamma_{ba} \delta_{ba}. \quad (C19) \]

The modified plane-wave expansion (B19) is used to express the exponential factor corresponding to the dot product in (C16), and the matrix element becomes

\[ M = N \sum_{a}^{N} \sum_{b}^{N} \left\langle \mathbf{l} \mathbf{L} \lambda \mathbf{l'} \mathbf{L'} \lambda' \right\rangle \tilde{\mathbf{r}}_{\mathbf{a}} \tilde{\mathbf{r}}_{\mathbf{a'}} \frac{4\pi \lambda}{2^L} \int d\mathbf{r} d\mathbf{R} \frac{1}{\mathbf{a} \mathbf{a'}} J_{\lambda} (2\xi \mathbf{R} \cdot \mathbf{r}) \times \int d\Omega_{\mathbf{r}} d\Omega_{\mathbf{R}} \left[ Y_{\lambda} (\mathbf{r}) \otimes Y_{\lambda} (\mathbf{R}) \right]^{*} \tilde{Y}_{\mathbf{l}} (\mathbf{r}) \tilde{Y}_{\mathbf{l'}} (\mathbf{R}), \quad (C20) \]

The integral over angles which is on the last two lines of (C20) is simplified by relation (B23) to

\[ I = (-1)^{l'} (1/4\pi) \sum_{\mathbf{K} \Lambda} \tilde{\mathbf{W}} (\mathbf{K}, \mathbf{L}, \mathbf{L'}, \mathbf{\lambda}, \mathbf{\lambda'}) \int d\Omega_{\mathbf{r}} d\Omega_{\mathbf{R}} \left[ Y_{\mathbf{l}} (\mathbf{r}) \otimes Y_{\mathbf{l'}} (\mathbf{R}) \right]^{*} Y_{\mathbf{l}} (\mathbf{r}) \tilde{Y}_{\mathbf{l'}} (\mathbf{R}) \]
The integrand in (C21) denoted by the symbol $A$ is written explicitly by employing the definitions of the tensor products:

$$A = \sum_{m}^{m} \left( \sum_{l}^{m} \left( \sum_{a}^{m} \left( \sum_{r}^{m} \left( \mathbf{r}_{a} \cdot \mathbf{Y}_{a} \mathbf{Y}_{a} \right) \mathbf{r}_{a} \cdot \mathbf{Y}_{a} \mathbf{Y}_{a} \right) \mathbf{r}_{a} \cdot \mathbf{Y}_{a} \mathbf{Y}_{a} \right) \mathbf{r}_{a} \cdot \mathbf{Y}_{a} \mathbf{Y}_{a} \right) \mathbf{r}_{a} \cdot \mathbf{Y}_{a} \mathbf{Y}_{a}$$

where the subscript attached to each $m$-value identifies the angular momentum to which the magnetic quantum number belongs.

Since the spherical harmonics are orthonormal, the integration over $\mathbf{r}_{a}$ gives $\delta_{m}^{m}$. Hence,

$$A = \sum_{m}^{m} \left( \sum_{l}^{m} \left( \sum_{a}^{m} \left( \sum_{r}^{m} \left( \mathbf{r}_{a} \cdot \mathbf{Y}_{a} \mathbf{Y}_{a} \right) \mathbf{r}_{a} \cdot \mathbf{Y}_{a} \mathbf{Y}_{a} \right) \mathbf{r}_{a} \cdot \mathbf{Y}_{a} \mathbf{Y}_{a} \right) \mathbf{r}_{a} \cdot \mathbf{Y}_{a} \mathbf{Y}_{a} \right) \mathbf{r}_{a} \cdot \mathbf{Y}_{a} \mathbf{Y}_{a}$$

The formula [110]

$$\int \mathbf{Y}_{1}^{*} \mathbf{Y}_{1} \mathbf{Y}_{2} \mathbf{Y}_{3} = \frac{1}{\sqrt{4\pi}} \delta_{13}$$

is applied in (C23) and the result is
A = \sum_{m_{La}}^{1} (M - m_{La} - m_{La}) (J M) (K^{M'-m_{La} - m_{La}}) (J' M') \\
\times (K^{M'-m_{La} - m_{La}}) (K^{M' - m_{La} - m_{La}}) (K^{010 - 10})(3/4\pi)^{1/2} K_{1}^{3} . \quad (C25)

From the Clebsch-Gordan coefficients, the selection rule

\[ m = M - M' \quad (C26) \]

is deduced.

The radial integral is essentially

\[ I_{R} = \int dr dR r^{a} \int \begin{array}{c}
\frac{1}{a} + L_{b} + L_{b} - T + 3 \\
\frac{1}{a} + L_{b} + L_{b} + T + 2
\end{array} R_{a} \exp(-\eta r^{2} - \zeta R_{a}^{2}) \frac{2}{\xi r} R_{a}, \quad (C27) \]

and can be performed by means of formula (B26) provided that the power of \( R_{a} \) can be written in the form \( 2m+\lambda \).

From the Clebsch-Gordan coefficients in (C21) and those in the Raynal-transformation coefficient derive the results (remembering that \( A = L_{a} \))

\[ K + L_{a} + \lambda = \text{even} , \quad (C28) \]
\[ L_{a} + L_{a} + \lambda = \text{even} , \quad (C29) \]
\[ L_{b} + L_{b} - T + 1 = \text{even} , \quad (C30) \]

and

\[ L_{a} + \tau = \text{even} . \quad (C31) \]
Adding (C29) and (31) gives

\[ L_a + \tau + \lambda = \text{even} \tag{C32} \]

Subtracting 2\( \lambda \) from the new result shows that

\[ L_a + \tau - \lambda = \text{even} \tag{C33} \]

which allows \( L_a + \tau \) to be written in the form \( 2m + \lambda \) with

\[ m = \frac{(L_a + \tau - \lambda)}{2} \tag{C34} \]

It is now necessary to show that \( 2m \geq 0 \), which is a condition on which formula (B26) depends. From one of the Clebsch-Gordan coefficients comes the triangle inequality

\[ |L_a - L'_a| \leq \lambda \leq L_a + L'_a \tag{C35} \]

from which is obtained

\[ -L'_a \leq L_a \lambda \tag{C36} \]

Adding \( \tau \) to both sides of (C36) yields

\[ \tau - L'_a \leq L_a + \tau - \lambda \tag{C37} \]

One of the Clebsch-Gordan coefficients in the
Raynal-transformation coefficient gives the triangle inequality

\[ |2\alpha - \tau| \leq \mu_a' \leq \tau, \quad (C38) \]

from which is deduced the result

\[ \tau - \mu_a' \geq 0. \quad (C39) \]

Comparing this result with (C37) gives the required condition, namely that

\[ \tau + \mu_a - \lambda \geq 0. \quad (C40) \]

Thus with \( 2m = \mu_a + \tau - \lambda \), the radial integral becomes

\[
I_R = \frac{\sqrt{\pi} \xi^\lambda m!}{4 \zeta^{m+\lambda+3/2}} \int \frac{r^{1+1+b+L-b-\tau+\lambda+3}}{r_a^4} \exp\left((\xi^2 - \eta \zeta) r_a^2 / \eta\right) \\
\times \frac{\lambda^{1/2}(-\xi^2 r_a^2 / \zeta)}{m}. \quad (C41) \]

The series expansion of \( L^{\lambda+1/2} \) given by expression (B40) is used, and (C42) becomes

\[
I_R = \frac{\sqrt{\pi} \xi \left(2m+2\lambda+1\right)!!}{4 \cdot 2^m \zeta^{m+\lambda+1/2}} \sum_{k=0}^{m} \left[ \frac{m}{k} \right] \frac{(2\xi^2 / \zeta)^k}{(2m+2\lambda+1)!!} \\
\times \int \frac{r^{1+1+b+L-b-\tau+\lambda+2k+3}}{r_a^4} \exp\left((\xi^2 - \eta \zeta) r_a^2 / \zeta\right). \quad (C42) \]

The integral in (C42) depends on whether the exponent of \( r_a \) is even or odd; this is now determined.
From the Clebsch-Gordan coefficient with vanishing projection quantum numbers in (C25) comes the result

\[ K + 1_a + 1 = \text{even}. \quad \text{(C43)} \]

Adding results (C28), (C30) and (C43) gives that

\[ 1_a + 1_b + L_b - \tau + \lambda + 1 = \text{even}. \quad \text{(C44)} \]

Hence

\[ 1_a + 1_b + L_b - \tau + \lambda + 2k + 3 = \text{even} = 2n. \quad \text{(C45)} \]

From (B8), the summation over \( \tau \) is between the limits

\[ 0 \leq \tau \leq 1_b + L_b. \quad \text{(C46)} \]

Therefore \( 2n \) is positive, and formula (B46) is applicable. The last line of (C42) gives the result

\[ \int \mathcal{R}_a = \frac{(2n-1)!!}{2[2(\eta \zeta - \xi^2)/\zeta]^n} \left( \frac{\pi \zeta}{\eta \zeta - \xi^2} \right)^{1/2}. \quad \text{(C47)} \]

Finally, the matrix element is

\[ \langle \phi_{K'}(b)_{J'M'} | r_a Y_{l_m}(\hat{r}_a) | \phi_{K}(a)_{J'M} \rangle = (\sqrt{3}/8)N_{a'b}(-1)^d \]

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\[ \times \sum_{1' L L' J} \left\langle 1' L' L' J | a a a b \right\rangle \hat{\mathcal{F}}_{a a a b} \left( K_{01} 0 | \lambda 0 \right) \left( L 0 L' 0 | \lambda 0 \right) \]

\[ \times W(K_{1 a a a a} | \lambda, \lambda) \frac{\lambda(2 m + 2 \lambda + 1)!}{2^{m+\lambda} \xi^{m+\lambda + 3/2}} \sum_{k=0}^{m} \binom{m}{k} \frac{(2 \xi^2 / \zeta)^k}{(2k + 2 \lambda + 1)!} \]

\[ \times \left( K / 1 a \right) \left( K_{01} 0 | 1 a \right) \frac{(2n-1)!}{2[2(\eta \xi - \xi^2) / \zeta]^{n}} \left[ \frac{\pi \xi}{\eta \xi - \xi^2} \right]^{1/2} \]

\[ \times \sum_{m} \left( \begin{array}{cc} 1 M - m & L_m a a a a \end{array} \right) \left( K_{m' - m} L_m a a a a | J' M' \right) \left( K_{m' - m} L_m a a a a | 1 M - m \right) \].

(C48)

It will be noticed that the subscripts \( k \) and \( k' \) do not appear explicitly in (C47); this is because - as explained in Chapter 7 - though both are convenient for ordering the basis functions in a linear fashion, they are not parameters upon which any quantities directly depend.

The several summations in (C47), with the exception of the one over \( k \), are determined by the limits allowed by the Clebsch-Gordan coefficients. Thus, the limits over \( K \) come from the parity Clebsch-Gordan coefficient in (C47). The limits with respect to \( 1' a \) and \( L' a \) are the same as are given in Appendix B, and may be further restricted by the Clebsch-Gordan coefficients introduced in subsequent analysis. Since all the Clebsch-Gordan coefficients have been given explicitly either in (C48) or in the expression for the Raynal transformation coefficient in Appendix
B, it is a routine exercise to derive all the limits by using the triangle inequality, and will not be pursued in detail here.

SECTION C4 - THE MATRIX ELEMENT OF $R_{1m} (R)$

The consideration of the matrix element

$$M = \langle \phi_{k_i(a)}(R) | R_{1m} (R) | \phi_{k_i(b)}(R) \rangle$$

(C49)

can proceed from (C21) if the angular integral is changed to

$$A = \int d\Omega d^2 \Omega \left[ Y_{1a} \hat{(r)} \hat{Y}_{1a} (R) \right]^* Y_{1a} (R) Y_{a} \hat{(r)} \hat{Y}_{a} (R)$$

and the radial integral in (C27) to

$$I_R = \int dr \int dR \int d\Omega \int d^2 \Omega \exp(-\eta r^2 - \xi R^2) Y_{a} \hat{(r)} \hat{Y}_{a} (R)$$

Explicitly, (C49) is given by

$$A = \sum_{m_1 m_2} (1 m_{1a} \lambda_{1a} M_{1a} | J_{M_{1a}} ) (K_{a_{1a}} \lambda_{1a} M_{1a} | J_{M_{1a}} ) \hat{Y}_{a_{1a}} (r) Y_{a} \hat{Y}_{a} (R)$$

(C50)

$$= \sqrt{(3/4\pi)} \sum_{m_{1a}} (1 m_{1a} \lambda_{1a} M_{1a} | J_{M_{1a}} ) (1 m_{1a} \lambda_{1a} M_{1a} | J_{M_{1a}} ) \hat{Y}_{a_{1a}} (r) \hat{Y}_{a} (R)$$

(C52)

The integration over $r_a$ in (C50) can be performed by means of formula (B26) with the variable of integration changed to $r_a$.
provided that the power can be written in the form $2m'\lambda$, with $m'$ an integer. To cast the exponent in this form, it is first noted that since now $K = \frac{1}{a}$, (C28) changes to

$$\frac{1}{a} + 1' + \lambda = \text{even}. \quad (C54)$$

Adding (C53) and (C30) yields

$$\frac{1}{b} + \frac{L_b}{b} - \tau + 1'_{a} + \lambda = \text{even}, \quad (C55)$$

and subtracting $2\lambda$ from the new result gives

$$\frac{1}{b} + \frac{L_b}{b} - \tau + 1'_{a} - \lambda = \text{even}. \quad (C56)$$

So indeed, the exponent can be written in the form $2m'\lambda$. The proof that it is a positive integer starts from one of the Clebsch-Gordan coefficients in the Raynal-transformation coefficient which vanishes unless

$$\left| 1'_{b} - 2\lambda - \frac{L_b}{b} + \tau \right| \leq 1'_{a} \leq 1 + \frac{L_b}{b} - \tau, \quad (C57)$$

from which results

$$\frac{1}{b} + \frac{L_b}{b} - \tau - 1'_{a} \geq 0. \quad (C58)$$

From the coefficient $\langle i_0'0'0 | \lambda0 \rangle$ comes the inequality

$$\left| 1 - 1' \right| \leq \lambda \leq 1 + 1', \quad (C59)$$

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from which is deduced

\[ l_a + l'_a - \lambda \geq 0. \tag{C60} \]

Combining (C57) and (C59) gives

\[ l_a + l_b + l'_b - \tau - \lambda \geq 0. \tag{C61} \]

Hence (B26) gives

\[
\int dr_a r_a^{2m'} \exp(-\zeta r_a^2) J_\lambda(2\xi r_a R_a) \\
\sqrt{\pi} m'! \frac{\xi^\lambda R_a^\lambda}{4 \eta^{m'+\lambda+3/2}} \exp\left(\xi^2 R^2/\eta\right) L_{m'}^{\lambda+1/2}(\xi^2 R^2/\eta), \tag{C62}
\]

where

\[ 2m' = l_a + l_b + l'_b - \tau - \lambda. \tag{C63} \]

Thus, with the use of the series expansion of \( L_{m'}^{\lambda+1/2} \) (B40),

\[
I_R = \sqrt{\pi} \frac{\xi^\lambda(2m'+2\lambda+1)!!}{4 \eta^{m'+\lambda+3/2}} \sum_{k'=0}^{m'} \frac{(m')!(2\xi^2/\eta)^k'}{(2k'+2\lambda+1)!!} \\
\times \int dR_a R_a^{l+\tau+2k'+\lambda+3} \exp\left((\xi^2-\zeta\eta)R_a^2/\eta\right). \tag{C64}
\]

It is necessary to determine whether the power of \( R_a \) is even or odd before the radial integral can be completely specified.
From the parity Clebsch-Gordan coefficient in (C52) derives the result

\[ \Lambda + l_a + 1 = \text{even} \quad \text{(C65)} \]

In order to arrive at (C49), the step involving formula (B23) had been used, and this supplies the result

\[ \Lambda + l'_a + \lambda = \text{even} \quad \text{(C66)} \]

Adding (C31), (C64) and (C65) gives that

\[ l_a + \tau + \lambda + 1 = \text{even} \quad \text{(C67)} \]

which shows that the exponent of \( R_a \) is even. Hence the integral over \( R_a \) is

\[ \int_{R_a} \frac{(2n'^{-1})!}{2[2(\eta \zeta - \xi^2)/\eta]^{n}} \left[ \frac{\pi \eta / (2n' a) / \eta} {\sqrt{2}} \right]^3, \quad \text{(C68)} \]

where

\[ 2n' = l_a + \tau + \lambda + 2k' + 3. \quad \text{(C69)} \]

The matrix element is

\[ \langle \phi_{K}^{(a)}_{jM} | \hat{R} Y_{a \lambda} (R) | \phi_{b}^{(b)}_{J_{M'}} \rangle = (\sqrt{3/8})(-1)^{j} N_{a b} \]

\[ \times \sum_{1' \Lambda} \langle \hat{1}_a b | \hat{1'} L \tau \lambda \rangle \langle \hat{a} \hat{a} | \hat{a} \hat{a} \rangle \langle \hat{a} \hat{a} | \hat{a} \hat{a} \rangle \]

\[ \langle \Lambda _1 | 0 \Lambda _0 | \lambda 0 \rangle \langle \Lambda _0 | 0 \Lambda _0 | \lambda 0 \rangle \]

\[ \sum_{1' \Lambda} \langle \hat{1}_a b | \hat{1'} L \tau \lambda \rangle \langle \hat{a} \hat{a} | \hat{a} \hat{a} \rangle \langle \hat{a} \hat{a} | \hat{a} \hat{a} \rangle \]

\[ \langle \Lambda _1 | 0 \Lambda _0 | \lambda 0 \rangle \langle \Lambda _0 | 0 \Lambda _0 | \lambda 0 \rangle \]
\[
\times W_{1_a 1'_a \lambda' a \lambda J} \frac{\xi^\lambda (2m'+2\lambda+1)!!}{2m' ! \eta} \frac{\sum_{k'} \left( k' \right) (2\varepsilon^2/\eta) k'!! \left( \Lambda/\ell \right)}{2[2(\eta\zeta-\xi^2)/\eta]^{1/2} \left( \eta \zeta - \xi^2 \right)} (\Lambda 010 | L 0)
\]

\[
\times \sum_{m'_{1a}} (1 m_{1a} M_{m_{1a}} | J'M') (1 m_{1a} A\lambda'_{m_{1a}} | J'M') (A\lambda_{m_{1a}} 1m_{1a} | M_{m_{1a}})
\]

(C70)

The final task is to show that in (C47) and (C67), the quantity \( \eta\zeta - \xi^2 \) is positive, a condition on which (B46) depends. From (C17) - (C19),

\[
\eta\zeta - \xi^2 = \left( \nu + \nu \gamma^2 + \lambda \gamma'^2 \right) \left( \lambda + \nu \delta^2 + \lambda \delta'^2 \right) - \left( \nu \gamma \delta + \lambda \gamma' \delta' \right)^2
\]

\[
= \nu \lambda \left( \gamma \delta' - \gamma' \delta \right)^2 + \nu \lambda + \nu \nu \delta^2 + \nu \lambda \delta'^2 + \nu \lambda \gamma^2 + \nu \lambda \gamma'^2
\]

Thus, this quantity is either zero or positive. From the Jacobi-coordinates inter-relations in Chapter 7, it is observed that \( \delta^2 = 1 \) always. As \( \nu_a \) and \( \nu_b \) never vanish, it follows that indeed, this quantity is positive.

Formula (C69) completes the specification of the dipole matrix element. It is clear from (C14) how expressions (C47) and (C69) are combined to obtain this quantity.
APPENDIX D - THE EXPRESSION FOR THE PROBABILITY DENSITY

In this appendix, the probability density is given with respect to the coordinates \( r_c \) and \( R_c \). The most useful value of \( c \) is 3. With the value of \( r_3 \) fixed and the angular dependence eliminated by integration, the expression facilitates the sort of plot which is familiar from the treatment of the hydrogen molecular ion in the framework of the Born-Oppenheimer approximation. Alternatively, a surface plot can be obtained by varying both \( r_c \) and \( R_c \).

The wavefunction is explicitly

\[
\psi_{JM} = \sum_c \sum_{a}^b \sum_{a}^L r_a^a R_a^a \exp(-\nu r^2 - \lambda R^2)[Y_1 (r) \hat{\otimes} Y_1 (R)]_{JM} \tag{D1}
\]

\[
\psi_{JM} = \sum_c \sum_{b}^b \sum_{b}^L r_b^b R_b^b \exp(-\nu r^2 - \lambda R^2)[Y_1 (r) \hat{\otimes} Y_1 (R)]_{JM} \tag{D2}
\]

The probability density is

\[
|\psi_{JM}|^2 = \sum_c \sum_{a}^b \sum_{a}^b r_a^a R_a^a r_b^b R_b^b \exp(-\nu r^2 - \lambda R^2 - \nu r^2 - \lambda R^2) \\
\times [Y_1 (r) \hat{\otimes} Y_1 (R)]_{JM} \quad [Y_1 (r) \hat{\otimes} Y_1 (R)]_{JM} \tag{D3}
\]
On using the Raynal transformation (B4) twice to change from coordinates \( b \) and \( a \) to \( c \), the result is

\[
|\psi_{JM}|^2 = (-1)^J \sum \sum \sum c^* c \langle 1_L J 1_L J \rangle a^a a^b a^a a^b b^b b^b c^c c^c \exp(-\eta R^2 - \zeta R^2)
\]

\[
\times \int d\Omega d\Omega \exp(-2\xi R) [Y_{1_L c} (r) \otimes Y_{1_L c} (R)]^* [Y_{1_L c} (r) \otimes Y_{1_L c} (R)]_{JM}
\]

with \( \eta, \zeta \) and \( \xi \) given by expressions (B16), (B17) and (B18). On using relation (B19) for the exponential function in the integrand, the probability density becomes

\[
|\psi_{JM}|^2 = (-1)^J 4\pi \sum \sum \sum c^* c \langle 1_L J 1_L J \rangle a^a a^b a^a a^b b^b b^b c^c c^c \exp(-\eta R^2 - \zeta R^2)
\]

\[
\times \int d\Omega d\Omega \exp(-2\xi R) [Y_{1_L c} (r) \otimes Y_{1_L c} (R)]^* [Y_{1_L c} (r) \otimes Y_{1_L c} (R)]_{JM}
\]

The integral over three spherical harmonics is given by (B24) and when this expression is inserted in (7.115), the probability density assumes the final form.
\[ |\psi_{JM}|^2 = (-1)^J \sum \sum \sum \sum c^* a_b a_b c^* N N \langle l_L l_j | l_L l_j \rangle a \rightarrow c \]

\[ \times \langle 1_b | 1_b | 1_b l_j' \rangle b \rightarrow c \]

\[ \times \int_{a^+ b^+ -T-T'}^{1_a + b^+ l_j'^T} \exp(-\eta r^2 - \zeta R^2) \]

\[ \times \mathcal{F} \left( 2\xi \xi \right) \]

\[ \mathcal{F} \left( 2\xi \xi \right) \] calculated from formula (7.54).
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