STUDY OF OSCILLATOR STRENGTHS AND DIPOLE SUM RULE USING A RELATIVISTIC NUCLEAR MODEL

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RULE USING A RELATIVISTIC NUCLEAR MODEL

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PREFACE

In this study, the dipole sum rule for the oscillator strengths has been evaluated using the non-relativistic harmonic oscillator model and the relativistic equivalent harmonic oscillator model. The results of the sum rules in both cases are not identical. The bremsstrahlung weighted cross section has also been calculated using the relativistic equivalent harmonic oscillator model and compared with the well known result obtained with the non-relativistic harmonic oscillator model. A relativistic correction factor for the bremsstrahlung weighted cross section has been evaluated.

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CHAPTER I

INTRODUCTION

The experimental discovery of the giant dipole resonance stimulated theoretical research in photo-nuclear reactions. While Goldhaber and Teller interpreted this in a unique way as a collective dipole vibration of the neutrons and protons in the nucleus, efforts were made to apply the knowledge of the well known atomic photo-effect to the nuclear gamma absorption. Levinger and Bethe made an extensive study of the dipole transitions in nuclei. Their study covered

a) oscillator strengths in the dipole approximation,

b) sum rule for these dipole oscillator strengths,

c) effect of neutron-proton exchange force on the sum rule,

d) cross section for photon absorption integrated over energy,

e) mean energy for photon absorption and a sum rule for quadruple transitions,

e) the dipole cross section weighted by the $\frac{dw}{w}$ approximation to the brumsstrahlung spectrum.

Before the work of Levinger and Bethe, Feenberg and Siegert showed that an attractive exchange force increased the summed oscillator strength above the value calculated on the basis of ordinary forces. Levinger and Bethe used an independent particle model of the nucleus, without Pauli Correlations between the nucleons, and established that quadrupole transitions are of negligible importance and that a suitable shell model of the nucleus and an application of time dependent perturbation theory to the nucleus-proton interaction can explain even the giant dipole resonance without invoking a special hydrodynamical model of collective mutual oscillations of neutron and proton fluids.

On the experimental side besides an extensive study of the giant resonant absorption, important contributions have been made in yields and angular distributions of γ-n processes, photoneutron cross sections, photodisintegration of very light nuclei and the brunsstrahlung weighted cross section. While there have been noticeable discrepancies in the measurements of different groups using different techniques, the agreement between theory and experiment has been fair but not of such a nature as to leave nothing to be desired. The Levinger-Bethe theory, revised by Levinger later, has been increasingly helpful in understanding photo-nuclear reactions. The existing theories are purely non-relativistic and it may well be that the non-existence of an exact relativistic nuclear model till now has prevented any consideration of relativistic motions of nucleons in their interaction with photons.

The Equivalent Harmonic Oscillator model recently proposed by Swamy and its application to the analysis of high energy electron scattering experiments by Braun, encourage investigation of its suitability in studying photo-nuclear cross sections. In this thesis two aspects of nuclear photon absorption have been studied, the validity of the sum rule for dipole transitions when relativistic effects are included, and secondly the improvement in the agreement between theory and experiment as far as brumsstrahlung weighted cross sections are concerned. The isotropic harmonic oscillator with spin-orbit coupling has long been used as a shell model of the nucleus. In particular Levinger used this model in his calculations. The EHO reduces to this in the non-relativistic limit, which facilitates comparisons and the study of relativity as a correction factor. While Levinger did make use of the Dirac-Coulomb wave functions to study relativistic radiative transitions in atoms, this has not been done for nuclei so far.

The viewpoint of this work is not to assume the existence of relativistic motions in nuclei but rather to ascertain regions of nuclei where relativistic motions may be significant if in such cases the relativistic theoretical results show a significant improvement in their agreement with experiment as compared with non-relativistic calculations.

CHAPTER II

OSCILLATOR STRENGTHS AND SUM RULE

The concept of oscillator strength and the sum rule orginated in the scattering of electromagnic waves by atoms, in particular the dispersion low developed by Kramers and Heisenberg[1] in quantum mechanics. In the same context Thomas and Kuhn[2] developed a sum rule for the oscillator strengths in the electric dipole approximation which was based on the correspondence principle. It is interesting to note that Heisenberg developed the most fundamental relations in quantum mechanics, the well-known quantum condition between x and P_x, $[x, P_x] = i\hbar$, based on the sum rule. In other words, the sum rule preceded quantum mechanics in a sense. For this reason it is necessary to trace the development of the concept of oscillator strengths and the sum rule.

In classical electrodynamics the total power radiated from an oscillating dipole is given by the expression[3]

$$P = \frac{ck^4}{3} |\vec{P}|^2 = \frac{\omega^4}{3c^3} |\vec{P}|^2 \qquad [1]$$

where, $\vec{P}$ is the oscillating dipole moment, c the speed of light, and ω the angular frequency.

This expression of course gives the total power radiated, whereas the angular distribution is given by the following expression,

$$\frac{dp}{d\Omega} = \frac{\omega^4}{8\pi c^3} |\vec{P}|^2 \sin^2\theta \qquad [2]$$

where the angle θ is measured from the direction of $\vec{P}$. In the derivation of these results in classical electromagnetic theory the energy of flux is given by Poynting's theorem and the power radiated per unit solid angle is averaged over a complete period of oscillation of the dipole.

Kramers[(4)] made the fundamental assumption that an atom, when exposed to radiation becomes a sourve of secondary spherical wavelets, which are coherent with the incident waves. A train of polarized harmonic waves of frequency ν, the electric vector of which at the point in space where the atom is saturated is represented by

$$\vec{E} = E\,\hat{n}\cos 2\pi\nu t \qquad [3]$$

is incident on the atom. E here is the amplitude and $\hat{n}$ is a unit vector. The secondary wavelets can be described as orginating from an oscillating dipole, the strength of which is given by

$$\vec{B} = P\,\hat{n}'\cos(2\pi\nu t - \phi) \qquad [4]$$

where P is the amplitude and $\hat{n}'$ also a unit vector, while ϕ represents the phase difference between the secondary and primary waves. The amplitude P will be proportional to the amplitude E of the incident waves, and this is the relationship that Kramers first calculated. Taking a model of the atom as an electron isotropically bound to a position of equilibrium, Kramers derived

$$P = E\,\frac{e^2}{m}\,\frac{1}{4\pi^2(\nu_1{}^2 - \nu^2)} \qquad [5]$$

where e and m are the charge and mass of an electron and ν_1 is one of the natural frequencies of the electron.

If $\nu_1 \nu_2 \ldots \nu_r$ are the absorbtion frequencies corresponding to the stationary states of the atom, then the formula becomes generalized to

$$P = E \sum_i f_i \frac{e^2}{m} \frac{1}{4\pi^2(\nu_i^2 - \nu^2)} \qquad [6]$$

and here f_i are constants which were actually determined experimentally from the absorption lines.

Modifying this classical picture by both the concept of stationary states and transitions between them, Kramers was able to derive the following formula, applying the correspondence principle that in the limit of large quantum numbers or as Planck's constant (h) tends to zero, the quantum mechanical system goes over into a classical system. Stated differently, in the region where successive stationary states of an atom differ only comparatively little from each other, the interaction between the atom and the field of radiation tends to coincide with the interaction to be expected on the basis of classical electrodynamic theory. The superscript a refer to absorbtion and the superscript e refers to emission in the following formula, the A's are the Einstein coefficients representing the probability of an isolated atom undergoing in unit time, transitions between stationary states giving rise to either emission or absorbtion of a spectral line.

$$P = E \sum_i A_i^a \tau_i^a \frac{e^2}{m} \frac{1}{4\pi^2(\nu_i^{a2} - \nu^2)} - E \sum_j A_j^e T_j^e \cdot$$

$$\cdot \frac{e^2}{m^2} \frac{1}{4\pi^2(\nu_j^{e2} - \nu^2)} \qquad [7]$$

A characteristic time t for both emission and absorption is introduced and this represents the time in which the energy of a particle performing linear harmonic oscillations of frequency ν is reduced to $1/\varepsilon$ of its value. A τ will be a dimensionless quantity f and this f represents the virtual oscillator strength. In the revised formula of Kramers, radiation reaction, that is the reaction of the atom on the incident radiation is taken into account by the introduction of virtual harmonic oscillators and it is the number or the strength of these oscillators that the f represents.

It is important to know that up to this point P represents the dipole moment induced by the electromagnetic wave that is incident on the atom and once the dipole moment is known the radiation is then computed according to the classical formula. The differential scattering cross section in classical theory is given by the ratio of the intensity of the radiation in a particular direction to the intensity of incident radiation.

When the atom is exposed to external monochromatic radiation of frequency ν it not only emits secondary monochromatic spherical waves of frequency ν which are coherent with the incident radiation but, according to the correspondence principle, spherical waves of other frequencies are also emitted, frequencies $(\nu \pm \nu')$, where $h\nu'$ denotes the energy difference of the atom between two stationary states. This incoherent radiation is the Raman effect in the atoms and molecules. Kramers and Heisenberg refined the original formulation of Kramers in a quantum mechanical but still semi-classical treatment of the interaction of the atoms and the radiation. The model of the atom is that of an oscillating dipole and the effort was to calculate the dipole moment induced in the atom by the incident electromagnetic wave. However, the possibility of incoherent scattered waves has been introduced and the formula for the scattering moment developed by Kramers and Heisenberg from the correspondence principle is given by

$$P(t) = E \frac{e^2}{4\pi^2 m} \left(\sum_a \frac{fa}{\nu_a^2 - \nu^2} - \sum_e \frac{fe}{\nu_e^2 - \nu^2} \right) \cdot \cos (2\pi\nu t) \qquad [8]$$

As in Kramer's original formula, once again, τ_ν is the decay time of classically oscillating electron with frequency ν

$$\tau_\nu = \frac{3c^3 m}{8\pi^2 e^2 \nu^2} \qquad [9]$$

and the strength of the transition is given by the number f

$$f = A \tau_\nu \qquad [10]$$

where A denotes Einstein's probability coefficient.

The total intensity of scattered light per unit time is given by the application of classical electrodynamic formula for the radiation from the oscillating dipole, using the above dipole moment.

It may be remarked incidentally that different types of scattered radiation and the transition between stationary states to which they give rise, should leave the energy distribution in the black-body radiation and statistical equilibrium distribution of the atoms unchanged.

Before proceeding to the fully quantum mechanical derivation of the well-known Kramers Heisenberg dispersion formula it is worth mentioning that Kuhn and Thomas[2] noticed a sum rule obeyed by the oscillator strengths corresponding to the above paragraph.

The quantum mechanical derivation of sum rule and the correspondence principle argument leads to the following set of formulas.

Lights of frequencies ν_1, $\nu_2 \ldots \nu_\gamma$ can induce transitions of the Hydrogen atom to a number of higher states ε_1, $\varepsilon_2 \ldots \varepsilon_\gamma$. For a radiation with frequency ν not close to one of the resonance frequencies ν_1, $\nu_2 \ldots \nu_2$ Thomas and Kuhn assumed that the oscillating dipole moment of the atom can be representing by

$$\frac{P}{E} = \frac{1}{4\pi^2} \frac{e^2}{m} \sum_{i=1}^{r} \frac{p_i}{\nu_i^2 - \nu^2} \qquad [11]$$

in analogy with classical dispersion theory. Here, as earlier, P and E are the amplitudes of the dipole moment and electric vector of the incident light respectively and p_i is the number of dispersion electrons which is appropriate for the transition $(o \to i)$ and which number is assumed identical with the number of absorption electrons.

For very large frequencies of incident radiation this reduces to

$$\frac{P}{E} = -\frac{e^2}{4\pi^2 m} \frac{1}{\nu^2} \sum_{i=1}^{r} p_i \qquad [12]$$

It is known that the dispersion associated with the dispersion vector $\vec{P}$ is equal to

$$-\frac{dE}{dt} = \frac{(2\pi\nu)^4}{3c^3} |\vec{P}|^2 \qquad [13]$$

and this simply gives the energy dispersed per unit time per atom as

$$-\frac{dE}{dt} = \frac{e^4}{3c^3 m^2} \cdot \left(\sum_{i=1}^{r} p_i\right)^2 E^2 . \qquad [14]$$

If one substitutes $\sum_{i=1}^{r} P_i = 1$ in this expression then the well-known cross section of Thomson is reproduced. It is this approximate agreement of the dispersion cross section with experiment that has established the validity of the rule $\sum_i P_i = 1$. The connection with optical dispersion relation however is given by a calculation, from the above induced dipole moment vector, of the dipole moment density or dipole moment per unit volume, and the polarizability and relating that to the refractive index. This of course is not the way in which the dispersion formula is useful for dispersion in quantum mechanics. The quantity of importance and interest, therefore, is the oscillator strength which in classical theory represents the number of dispersion electrons that participate in the proper vibration in question. In quantum theory this number need not be an interger, it represents the strength of the oscillator or what fraction of a given electron trated as a classical oscillator contributes to the dispersion. By comparison of the formulas of Kramers and Kuhn it is easily noticed that the oscillator strength f used by Kuhn is $(A\tau)$ introduced by Kramers namely the product of the Einstein's coefficient and the decay time of electron. The Kramers Heisenberg derivation is not fully quantum mechanical not only because it was still obtained from the correspondence principle way of calculating the dipole moment, but the oscillator strengths are not given in terms of quantum mechanical matrix elements and most important of all the radiation field is not quantized. As is well-known, the most accurate description of the interaction of matter and radiation involves quantizing the radiation field and treating the interaction between radiation and atoms as a perturbation. The transition probabilities and the cross section are then calculated according to time dependent perturbation theory. The perturbing Hamiltonian is

$$H_{int} = -\frac{e}{\mu}(\vec{P} \cdot \vec{A}) + \frac{e^2}{2\mu} A^2 \qquad [15]$$

and the radiation field is quantized. One speaks not of electromagnetic waves being scattered by the atom but of photons and electrons and the photon number and electron number before and after the collision. In the case of dispersion therefore there are two possibilities which experiments can not distinguish. A quantum of energy $h\nu$ and momentum $\frac{h\nu}{c}$ is obsorbed by the atom or, more precisely by the electron in the coulomb field. So in an intermediate state no light quantum is present. The excited electron then makes the transition to the final state and a photon with energy $h\nu'$ is emitted. On the other hand it is equally possible that in the field of the incident photon the electron first emitted a $h\nu'$, thus creating a intermediate state in which two light quanta $h\nu$, $h\nu'$ are present and eventually the electron absorbs the incoming radiation $h\nu$. There is a possibility of interference between these two processes and therefore the matrix elements have first to be added and then the absolute square of their sum is introduced into the formula of the time dependent perturbation theory for the transition probability. The matrix elements are computed in the basis of product wave functions, the factors of which represent the wave functions of the photon and the electron in the initial and the final states. The vector potential in the interaction Hamiltonial given above is usually taken to be

$$\vec{A} = A_o \, \hat{\varepsilon} \, e^{-i \, \vec{k} \cdot \vec{r}} \qquad [16]$$

The time factor is omitted here and is taken into account by the energy conservation between the two stationary states and the photon. This leads to $\vec{P} \cdot \vec{A}$ being equal to

$$\vec{P} \cdot \vec{A} = A_o \, (\vec{p} \cdot \hat{\varepsilon}) \, e^{-i \, \vec{k} \cdot \vec{r}} \qquad [17]$$

The presence of the exponential factor, often referred to as a retardation factor, complicates the evaluation of the integrals. However, in the cases of experimental interest (kr) happens to be a very small quantity being the ratio of the linear dimension of the atom (10^{-8} cm) and the wave length of the outgoing radiation (4000×10^{-8} cm). In this long wave length approximation, therefore, the $e^{-i \, \vec{k} \cdot \vec{r}}$ can be replaced by 1 and this is often referred to as a dipole approximation, because then the quantum mechanical formula parallels the oscillating dipole in the Kramers Heisenberg formulation of dispersion theory. This fully quantum mechanical formula is given in Heitler's Quantum Theory of Radiation(5)

$$d\phi = r_o^{\,2} \frac{k}{k_o} \, d\Omega \, \Big[\frac{1}{\mu} \sum_i \Big(\frac{P_{o} n_o n_i \, P n_i n}{E_o - E_i + k_o} + \frac{P n_o n_i \, P_o n_o n}{E_o - E_i - k}\Big) + \delta n n_o \cos \theta\Big]^2 \qquad [18]$$

and in the case of coherent scattering

$$d\phi = r_o^{\,2} \, d\Omega \, \Big[\frac{1}{\mu} \sum_i \Big(\frac{P_o n_o n_i \, P n_i n_o}{E_o - E_i + \kappa_o} + \frac{P n_o n_i \, P_o n_i n_o}{E_o - E_i - k_o}\Big) + \cos \theta\Big]^2 \qquad [19]$$

In the above formula if $n_o = n$ then it corresponds the Rayleigh scattering, wherein the process of scattering the quantum state of the atom is not changed. If $n_o \neq n$ then the atom has made a transition and this corresponds to Raman scattering, where the incident photon and the outgoing photon have different frequencies and the difference in energy is used up in making a jump between stationary states by the atom on which the light is incident.

We now can introduce the fully quantum mechanical definition of the oscillator strength from the above formula. The oscillator strength is as proportional to the numerator of the two terms in the cross section formula.

$$f_{nn'} = \frac{2m}{\hbar} \omega_{n'n} \left| \langle n | z | n' \rangle \right|^2 \qquad [20]$$

This is the definition of the oscillator strength in the dipole approximation of the quantum mechanical interaction between radiation and matter. And the most important sum rule Thomas-Reiche-Kuhn rule is now a rule for the sum of the oscillator strength for all transitions which start from a definite state n of the atom. This happens to be a very general rule which holds for any atom or molecule with or without external fields, for any polarization direction and no matter which (if any of the various angular momentum operators are constants of the motion). For one electron this sum equals one and for z electrons this sum is equal to the total number of electrons z. Stated simply, this sum is

$$\sum_{n'} f_{n'n} = z \qquad [21]$$

(sometimes the notation $f_n^{n'}$ is also used for $f_{n'n}$). Although it has been established in accordance with the correspondence principle by Thomas and

Kuhn the sum rule can be derived simply by considering the following commutator relations and using the properties of completeness of the eigenfunctions of a Hermitean Hamiltonian, and closure.

Consider the double commutator $[[z, \underset{\sim}{H}], z]$. If $\underset{\sim}{H} = \frac{1}{2m}\vec{P}^2 + V(r)$, then according to Heisenberg matrix mechanics we have, because $[z, V(r)] = 0$,

$$[z, \underset{\sim}{H}] = \frac{1}{2m}[z, P_z^{\ 2}] = \frac{i\hbar}{m} P_z \qquad [22]$$

using the quantum condition $[z, P_z] = i\hbar$ and $[z, P_x] = [z, P_y] = 0$, we have

$$[[z, \underset{\sim}{H}], z] = [\frac{i\hbar}{m} P_z, z] = \frac{\hbar^2}{m} \qquad [23]$$

Taking the expectation value of both sides with respect to the normalized eigenstate $|0\rangle$ of the Hamiltonian $\underset{\sim}{H}$,

$$\langle 0|[[z, H], z]|0\rangle = \frac{\hbar^2}{m}\langle 0||0\rangle = \frac{\hbar^2}{m} \qquad [24]$$

The left hand side equals

$$\sum_n \left\{ \langle 0|[z, H]|n\rangle\langle n|z|0\rangle - \langle 0|z|n\rangle\langle n|[z, H]|0\rangle \right\} \qquad [25]$$

Now

$$\langle 0|[z, H]|n\rangle = \langle 0|zH|n\rangle - \langle 0|Hz|n\rangle \qquad [26]$$

$$H|n\rangle = E_n|n\rangle \qquad [27a]$$

$$\langle 0|H = E_0\langle 0| \qquad [27b]$$

$$\langle 0|[z, H]|n\rangle = (E_n - E_0)\langle 0|z|n\rangle \qquad [28]$$

therefore,

$$\langle 0|[[z, H], z]|0\rangle = 2\sum_n (E_n - E_o)|\langle 0|z|n\rangle|^2 \quad [29]$$

Hence the sum rule,

$$\sum_n f_{on} = \frac{2m}{\hbar^2} \sum_n (E_n - E_o)|\langle 0|z|n\rangle|^2$$
$$= \frac{2m}{\hbar^2} \cdot \frac{\hbar^2}{2m} = 1 \quad [30]$$

Two things are very important in the above derivation, firstly that the double commutator is equal to $(\frac{\hbar^2}{m})$ and secondly the matrix elements of P are related to the matrix elements of Υ through the Bohr frequency condition. We will later see that these relations are not necessarily valid in the case of a relativistic theory of electron, viz, if $\underset{\sim}{H}$ happens to be a Dirac Coulomb Hamiltonian instead of a non-relativistic Schrödinger Hamiltonian for central fields.

The quantum mechanical T. R. K. sum rule can be said to correspond to classical integrated power absorbtion for forced oscillation by a charged oscillator or that it gives the classical Thomson cross section for the forward scattering amplitude.

A third interpretation of the oscillator strength is through the quantum mechanical expression for the electric polarizability.

$$\frac{\text{dipole moment}}{\text{electric field}} = 2e^2 \sum_n \frac{|\langle n|z|0\rangle|^2}{E_n - E_o}$$
$$= e^2 \sum_n \frac{f_{on}}{m\,\omega_{on}^2} \quad [31]$$

Here the oscillator strength is the fraction of the electron bound by a linear sping of spring constant $\kappa_{on} = m\,\omega_{on}^2$.

We will now calculate the oscillator strength for nuclear case, i.e., γ-ray absorbtion by nuclei. It is to be noticed that as far as the physics and the quantum mechanical analysis are concerned, the absorbtion of optical photons by atoms and absorbtion of gamma rays by nuclei are two similar processes, and it is in this way that Bethe and Levinger applied the knowledge of atomic spectra to nuclear photon absorbtion. The model of the nucli will be a shell model in which each nucleon is moving independently of the others in an average central field described by an astropic harmonic oscillator potential. The energy levels are given by E_n, Eq. [32] $E_n = \hbar\omega_c\ (2v + \ell + \frac{3}{2})$ and the normalized single particle wave functions are given by $U_{vlm}(r.\theta.\phi.)$

$$U_{v\ell m} = R_{v\ell}(r)\, Y_\ell^m(\theta,\phi) \qquad [33]$$

$$R_{v\ell}(r) = \left\{\frac{2\lambda^2\, \Gamma(v+\ell+\frac{3}{2})}{v!\,[\Gamma(\ell+\frac{3}{2})]^2}\right\}^{\frac{1}{2}} (\lambda r)^\ell\, e^{-\frac{1}{2}\lambda^2 r^2}\ {}_1F_1\left(\begin{matrix}-v \\ \ell+\frac{3}{2}\end{matrix};\lambda^2 r^2\right)$$

$$= \left\{\frac{2\lambda^2\, \Gamma(v+\ell+\frac{3}{2})}{v!\,[\Gamma(\ell+\frac{3}{2})]^2}\right\}^{\frac{1}{2}} \chi^{-\frac{3}{4}}\, M_{v+\frac{1}{2}+\frac{3}{4},\,\frac{\ell}{2}+\frac{3}{4}}(\chi)$$

[34]

where, M is a Whittaker function and λ represents the oscillator constant $\sqrt{\frac{m\omega}{\hbar}}$ and $\chi \equiv \lambda^2\gamma^2$. These solutions have a definite parity $(-)^\ell$.

This Hamiltonian has rotational symmetry writing z as $r\cos\theta = \sqrt{\frac{4\pi}{3}}\, rY_1^0$ we get the parity selection rule for the matrix element of z, by considering the following integral:

$$\int Y_{\ell_3}^{m_3 *}\, Y_{\ell_2}^{m_2}\, Y_{\ell_1}^{m_1}\, d\Omega = \left\{\frac{(2\ell_1+1)(2\ell_2+1)}{4\pi(2\ell_3+1)}\right\}^{\frac{1}{2}} C_{m_1 m_2 m_3}^{\ell_1 \ell_2 \ell_3}\, C_{0\,0\,0}^{\ell_1 \ell_2 \ell_3} \qquad [35]$$

In our case $\ell_1 = \ell$, $\ell_2 = 1$, $\ell_3 = \ell'$ and $m_1 = m$, $m_2 = o$ and $m_3 = m'$. The Clebsch-Gordan (c-) coefficients vanish whenever $\ell' \neq \ell + 1$ or $\ell - 1$ $m' \neq m$.

The selection rule for the magnetic quantum number (m) is, therefore,

$$\Delta m \equiv m' - m = o \qquad [36]$$

The selection rule for the orbital quantum number (ℓ) is, therefore,

$$\Delta \ell \equiv \ell' - \ell = \pm 1 \qquad [37]$$

and

$$\langle v' \ \ell{+}1 \ m | z | v \ \ell \ m \rangle = \sqrt{\frac{(\ell+1)^2 - m^2}{(2\ell+3)(2\ell+1)}} \langle v' \ \ell{+}1 | r | v \ \ell \rangle \qquad [38a]$$

$$\langle v' \ \ell{-}1 \ m | z | v \ \ell \ m \rangle = \sqrt{\frac{\ell^2 - m^2}{(2\ell+1)(2\ell-1)}} \langle v' \ \ell{-}1 | r | v \ \ell \rangle \qquad [38b]$$

$$\langle v' \ \ell' \ m | z | v \ \ell \ m \rangle = 0$$

for all other ℓ'. [38c]

And the radial integral in the oscillator strengths becomes

$$\langle v' \ \ell{+}1 | r | v \ \ell \rangle = \int R_{v'\ell+1}(r) \, R_{v\ell}(r) \, r^3 \, dr$$

$$= \left\{ \frac{2\lambda^3 \, \Gamma(v + \ell + \frac{3}{2})}{v! \, [\Gamma(\ell + \frac{3}{2})]^2} \right\}^{\frac{1}{2}} \left\{ \frac{2\lambda^3 \, \Gamma(v' + \ell + \frac{5}{2})}{v'! \, [\Gamma(\ell + \frac{5}{2})]^2} \right\}^{\frac{1}{2}} \frac{1}{2\lambda^4} \times$$

$$\times \int x^{-\frac{1}{2}} M_{v+\frac{l}{2}+\frac{3}{4},\, \frac{l}{2}+\frac{1}{4}}(x)\, M_{v'+\frac{l}{2}+\frac{5}{4},\, \frac{l}{2}+\frac{3}{4}}(x)\, dx$$

Evaluating the integral(10), we get

$$\langle v'\, l+1 | r | v\, l \rangle = \frac{1}{\lambda} \left\{ \frac{\Gamma(v+l+\frac{3}{2})\, \Gamma(v'+l+\frac{5}{2})}{\Gamma(v+1)\, \Gamma(v'+1)} \right\}^{\frac{1}{2}} \times$$

$$\times \frac{(-1)^{v+v'}}{\Gamma(l+\frac{3}{2})\, \Gamma(l+\frac{5}{2})} \cdot \frac{\Gamma(l+\frac{3}{2})\, \Gamma(l+\frac{5}{2})\, \Gamma(l+\frac{5}{2})\, \Gamma(v+1)}{\Gamma(v'+l+\frac{5}{2})\, \Gamma(v-v'+1)}$$

$$\times \sum_{m=0}^{1} \binom{1}{m} \binom{v'}{v-m} \frac{\Gamma(1+m)}{\Gamma(l+m+\frac{3}{2})}$$

$$= (-1)^{v+v'} \frac{1}{\lambda} \left\{ \frac{\Gamma(v'+1)\, \Gamma(v+l+\frac{3}{2})}{\Gamma(v+1)\, \Gamma(v'+l+\frac{5}{2})} \right\}^{\frac{1}{2}} \times$$

$$\times \frac{1}{\Gamma(v-v'+1)\, \Gamma(v'-v+2)} \cdot \left\{ (l+\frac{3}{2})(v'-v+1) \right.$$

$$\left. + v \right\} \qquad [39]$$

From the above formula we get by algebraic manipolation the following oscillator strengths.

$$f_{v\,l\,m}^{v\;l-1\;m} = (-) \frac{2\mu}{\hbar^2} \hbar\omega_c \frac{1}{\lambda^2} (v+l+\tfrac{1}{2}) \frac{l^2-m^2}{(2l+1)(2l-1)} \qquad [40a]$$

$$f_{v\,l\,m}^{v+1\;l-1\;m} = \frac{2\mu}{\hbar^2} \hbar\omega_c \frac{1}{\lambda^2} (v+1) \frac{l^2-m^2}{(2l+1)(2l-1)} \qquad [40b]$$

$$f_{v\ell m}^{v\,\ell+1\,m} = \frac{2\mu}{\hbar^2}\hbar\omega_c\frac{1}{\lambda^2}\left(v+\ell+\frac{3}{2}\right)\frac{(\ell+1)^2-m^2}{(2\ell+3)(2\ell+1)} \qquad [40c]$$

$$f_{v\ell m}^{v-1\,\ell+1\,m} = (-)\frac{2\mu}{\hbar^2}\hbar\omega_c\frac{1}{\lambda^2}(v)\frac{(\ell+1)^2-m^2}{(2\ell+3)(2\ell+1)} \qquad [40d]$$

As a result of the selection rules on the quantum numbers v, ℓ and m, in the summation only a few terms survive namely $v' = v,\ v+1$ for $\ell' = \ell+1$ and $v' = v_1\ v-1$ for $\ell' = \ell - 1$. Incidentally it is to be noted that the summation, as far as the sum rule is concerned, has to be done on all the quantum numbers which represent a particular state of a one particle system. Carrying out this summation

$$\sum_{n'} f_{n'n} = f_{v\ell m}^{v\,\ell-1\,m} + f_{v\ell m}^{v+1\,\ell-1\,m} + f_{v\ell m}^{v\,\ell+1\,m} + f_{v\ell m}^{v-1\,\ell+1\,m} = 1 \qquad [41]$$

We therefore get the sum equal to 1. This is not unexpected because the solutions form a complete set and are the eigenfunctions of the non-relativistic Hamiltonian

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2} m\, w_o^{\,2} r^2 \qquad [42]$$

and therefore the double commutator relation Eq. (23), and the replacement of P matrix element by the γ matrix element are easily accomplished. However, this calculation provides an algebric and numerical check on the accuracy of the sum rule. It is pointed out by Fock[18] that the sum rule is really not valid if one goes to a more complicated system than Hydrogen atom. It is generally understood that if there are z electrons the sum of the oscillator strength gives z. This really does not turn out to be the case if one bears in mind the identity of the electrons and that they obey the Pauli exclusion principle. The requirement of antisymmetry on the wave function of the many electron system results in the peculiar quantum mechanical effect of an exchange integral. The single particle Hamiltonian should really be written as the sum of three terms, the kinetic energy, potential energy and the exchange energy which has a sign opposite to the potential energy. With this Hamiltonian, the double commutator relation, which is the most important quantum mechanical equation that gives rise to the sum rule, is no longer the same because z in general will not commute with the exchange part of the Hamiltonian. In the case of the nuclear photo effect Levinger and Bethe corrected the sum rule for certain other reasons because in their original treatment they ignored the Pauli correlations. The two particle nuclear force has, besides the ordinary interaction, an exchange interaction. This exchange interaction is a dynamical part of the nuclear force and is not to be confused with a quantum mechanical exchange arising from the antisymmetry of the wave function, i.e., arising from the Pauli positional correlations in the motions of the particles. They noticed that the final result of the sum rule has to be corrected[7]

$$\sum_n f_{on} = \frac{NZ}{A}(1 + 0.8\chi) \qquad [43]$$

where N is the number of neutrons and Z the number of protons and A is the sum of Z and N. χ is the fraction of attractive force for the neutron-proton potential. In spite of this, however, the sum rule has been very helpful in understanding photo nuclear reactions. The most outstanding photo nuclear reaction happens to be the gaint dipole resonance which is known to exist in almost all nucli except the really light ones. In the analysis of this resonant photo absorbtion the sum rule plays an important part.

The above discussion is confined to non-relativistic quantum mechanics. It is interesting to ask what happens to the sum rule if in the computation of the oscillator strength, instead of non-relativistic basis sets, relativistic basis sets are used. This has never been attempted because of the unavailability of a relativistical single particle nuclear model. Very recently a relativistic equivalent harmonic oscillator model has been proposed[8]. It is therefore tempting to use the exact relativistic eigenfunctions of this Hamiltonian to compute, as an approximation, the oscillator strengths and the sum rule. While a detailed discussion of the relativistic oscillator is given in a later chapter, the important equations and results will be reproduced here. The eigenfunctions of the Hamiltonian happen to be

$$\Psi_{v\chi\mu} = \left\{ 1 + \frac{(E - m_0)^2}{4\lambda^2 (v + |\chi| + \frac{1}{2})} \right\}^{-\frac{1}{2}} \begin{pmatrix} |v \chi \mu\rangle \\ \dfrac{S_\chi (E - m_0)}{2\lambda\sqrt{v + |\chi| + \frac{1}{2}}} |v -\chi \mu\rangle \end{pmatrix} \quad [44]$$

It is interesting to note that the radial functions occurring in this spinor are identical to the functions occurring in the non-relativistic harmonic oscillator solutions. Secondly, this relativistic Hamiltonian goes over into the non-relativistic Hamiltonian in the limit of low velocities. This facilitates greatly the comparison between relativistic and non-relativistic results and, in particular, the evaluation of the relativistic corrections, if any, that need to be made both in the oscillator strengths as well as the sum rule.

The Dirac quantum number χ in the eigenfunction $\Psi_{v\chi\mu}$ can be expressed in the language of orbital quantum number ℓ using the relation in Eq. (52) and, therefore, the eigenfunction $\Psi_{v\chi\mu}$ can be written as function of quantum number v, ℓ, and μ for a chosen j (or χ) value as in Eq. (70). The parity selection rules for the matrix element of z, derived for the Spherical Harmonics $Y_\ell^m(\theta.\phi)$ as in Eq. (36), Eq. (37) and Eq. (38) can now be applied, to simplify the integrals and further the radial integrals are the same as given in Eq. (39). The latter happens to be so because the radial parts of the wave functions in the relativistic and non-relativistic cases are the same. The oscillator strengths calculated using the eigenfunctions of E. H. O. Hamiltonian are now formed as follows: When initial state is chosen such that $j = \ell + \frac{1}{2}$ ($\kappa < o$), then, for $j' = \ell' + \frac{1}{2}$ ($\chi' < o$) we have

$$f_n^{n'} = f_{v\chi\mu}^{v\,\chi-1\,\mu} = \frac{2m}{\hbar^2}\left(E_n - E_{n'}\right)\frac{1}{\lambda^2\,(2\ell+3)^2} \times$$

$$\times \frac{(\ell+\mu+\frac{3}{2})(\ell-\mu+\frac{3}{2})}{4\left(E_n^2 - m_oc^2E_n\right)\left(E_{n'}^2 - m_oc^2E_{n'}\right)}$$

$$\times \Big\{ 4\lambda^2\hbar^2c^2\,(v+\ell+\tfrac{3}{2})\sqrt{v+\ell+\tfrac{5}{2}} +$$

$$(E_n - m_oc^2)(E_{n'} - m_oc^2)\sqrt{v+\ell+\tfrac{5}{2}}\Big\}^2 \qquad [45a]$$

$$f_n^{n'} = f_{v\chi\mu}^{v\,\chi+1\,\mu} = \frac{2m}{\hbar^2}(E_n - E_{n'})\frac{1}{\lambda^2\,(2\ell+1)^2} \times$$

$$\times \frac{(\ell+\mu+\frac{1}{2})(\ell-\mu+\frac{1}{2})}{4(E_n^2 - m_0c^2 E_n)(E_{n'}^2 - m_0c^2 E_{n'})}$$

$$\times \Big\{ 4\lambda^2\hbar^2c^2\,(v+\ell+\tfrac{1}{2})\sqrt{v+\ell+\tfrac{3}{2}} +$$

$$(E_n - m_0c^2)(E_{n'} - m_0c^2)\sqrt{v+\ell+\tfrac{3}{2}}\Big\}^2$$

[45b]

and for $j' = \ell - \frac{1}{2}$ we have

$$f_n^{n'} = f_{v\chi\mu}^{v-1\,-\chi\,\mu} = \frac{2m}{\hbar^2}(E_n - E_{n'})\frac{1}{\lambda^2\,(2\ell+1)^2} \times$$

$$\times \frac{1}{4(E_n^2 - m_0c^2 E_n)(E_{n'}^2 - m_0c^2 E_{n'})}$$

$$\times \frac{4\mu^2 v\,(4\lambda^2\hbar^2c^2)^2\,(v+\ell+\frac{3}{2})(v+\ell+\frac{1}{2})}{(2\ell+3)^2}$$

[45c]

$$f_n^{n'} = f_{v\chi\mu}^{v+1\,-\chi\,\mu} = \frac{2m}{\hbar^2}(E_n - E_{n'})\frac{1}{\lambda^2\,(2\ell+3)^2}$$

$$\times \frac{(\ell+\mu+\frac{3}{2})(\ell-\mu+\frac{3}{2})}{4(E_n^2 - m_0c^2 E_n)(E_{n'}^2 - m_0c^2 E_{n'})} \times$$

$$\times \frac{4\mu^2(v+1)\,(E_n-m_oc^2)^2\,(E_{n'}-m_oc^2)^2}{(l+\mu+\frac{3}{2})\,(l-\mu+\frac{3}{2})\,(2l+1)^2}$$

[45d]

$f_n^{n'}$ = o for all other cases.

Then the sum rule

$$\sum_{n'} f_{n'n} = \sum_{v'}\sum_{\chi'}\sum_{\mu'} f_{v\chi\mu}^{v'\chi'\mu'}$$

$$= \frac{2m}{\hbar^2}\,\frac{(E_n-E_{n_1'})\,(l+\mu+\frac{3}{2})(l-\mu+\frac{3}{2})}{4\,(E_n^2-m_oc^2E_n)(E_{n_1'}^2-m_oc^2E_{n'})\,\lambda^2(2l+3)^2}$$

$$\times\Big\{16\,\lambda^4\hbar^4c^4\,(v+l+\tfrac{3}{2})^2(v+l+\tfrac{5}{2}) + 8\lambda^2\hbar^2c^2$$

$$\times(v+l+\tfrac{3}{2})(v+l+\tfrac{5}{2})\,(E_n-m_oc^2)(E_{n_1'}-m_oc^2)$$

$$+(E_n-m_oc^2)^2\,(E_{n_1'}-m_oc^2)^2(v+l+\tfrac{5}{2})$$

$$+\frac{4\mu^2(v+1)\,(E_n-m_oc^2)^2(E_{n_1'}-m_oc^2)^2}{(l+\mu+\frac{3}{2})(l-\mu+\frac{3}{2})(2l+1)^2}\Big\}$$

$$+\frac{2m}{\hbar^2}\,\frac{(E_n-E_{n_2'})(l+\mu+\frac{1}{2})\,(l-\mu+\frac{1}{2})}{4(E_n^2-m_oc^2E_n)\,(E_{n_2'}^2-m_oc^2E_{n_2'})\,\lambda^2(2l+1)^2}$$

$$\times\Big\{16\,\lambda^4\hbar^4c^4\,(v+l+\tfrac{1}{2})^2(v+l+\tfrac{3}{2}) + 8\lambda^2\hbar^2c^2\,\times$$

$$\times (v+l+\tfrac{1}{2})(v+l+\tfrac{3}{2})(E_n-m_oc^2)(E_{n'_2}-m_oc^2)$$

$$+ (E_n-m_oc^2)^2(E_{n'_2}-m_oc^2)^2(v+l+\tfrac{3}{2})$$

$$+ \left.\frac{4\mu^2 v(4\lambda^2\hbar^2c^2)^2(v+l+\tfrac{3}{2})(v+l+\tfrac{1}{2})}{(l+\mu+\tfrac{1}{2})(l-\mu+\tfrac{1}{2})(2l+3)^2}\right\}$$

[46]

Because of the functional dependence of the terms on the energy E_v of the state it is obvious that the terms can not be summed as easily as in the non-relativistic case. This is done numerically and the sum gives 0.68 as against 1 in the non-relativistic case. The detail of the choice of λ, the oscillator parameter, is discussed elsewhere. This result, although it compares with Levinger's[11] result of 0.85 for the Coulomb field case (Levinger, incidentally includes retardation also), is approximate because of the nature of the derivation. For a realistic theory the interaction of the proton with the electromagnetic field has to be treated according to quantum electrodynamics. This is done in a later chapter.

CHAPTER III

THE RELATIVISTIC EQUIVALENT HARMONIC OSCILLATOR

As a preliminary to the introduction of the relativistic Equivalent Harmonic Oscillator proposed by Swamy[8] it is necessary to discuss the spin angle functions. The spherical harmonics which form an orthonormal set of functions in polar angle space are defined as

$$Y_\ell^m(\theta,\varphi) = (-)^m \sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}}\ \sin^m\theta \frac{d^m}{d(\cos\theta)^m} P_\ell(\cos\theta) e^{im\varphi} \quad [47]$$

These satisfy the phase relation

$$Y_\ell^{-m} = (-1)^m Y_\ell^{m*} \quad [48]$$

and the orthonormal property

$$\int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\varphi\, Y_{\ell'}^{m'*}(\theta,\varphi) Y_\ell^m(\theta,\varphi) = \delta_{\ell\ell'} \delta_{mm'} \quad [49]$$

The well known spin functions for a particle of spin 1/2 are given by

$$\chi_{\frac12}^{\frac12} \to \alpha = \binom{1}{0} \ ; \quad \chi_{\frac12}^{-\frac12} \to \beta = \binom{0}{1} \quad [50]$$

with the spin up or down $m_s = \pm \frac12$ is taken along the Z axis. From these two the spin-angle functions are now defined as

$$\chi_x^\mu = \sum_{\substack{\tau \\ \tau = \pm\frac12}} C_{\mu-\tau\ \tau\ \mu}^{\ell\ \frac12\ j}\, Y_\ell^{\mu-\tau} \chi_{\frac12}^{\tau} \quad [51]$$

where C are Clebsch-Gordan coefficients. These were also called spherical spinors by Rose and Biedenharn who first introduced them[9]. In the above, the Dirac quantum number κ simultaneously determines both 1 and j the latter being the usual total angular momentum quantum number relating to the quantum mechanical vector sum of the orbital angular momentum and spin. This is an algebraic number which can take on all integral values except 0. It is negative if the spin and orbital angular momenta are parallel and positive in the other case. We thus have

$$\begin{aligned} &\text{for} \quad j = \ell - \tfrac{1}{2} \;, \quad \kappa = \ell \\ &\text{for} \quad j = \ell + \tfrac{1}{2} \;, \quad \kappa = -\ell - 1 \end{aligned} \qquad [52]$$

1 now can be treated as a function of κ and one introduces $1(-\kappa)$, denoted by the symbol $\bar{\ell}$, as follows

$$\begin{aligned} &\text{for} \quad j = \ell - \tfrac{1}{2} \;, \quad \bar{\ell} = \ell - 1 \\ &\text{for} \quad j = \ell + \tfrac{1}{2} \;, \quad \bar{\ell} = \ell + 1 \end{aligned} \qquad [53]$$

We note that in either case $|\kappa| = j + 1/2$. For each κ there will be $2|\kappa|$ values of μ which can take on the half integral values:

$$\mu = \pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}, \ldots, \pm(|\kappa| - \tfrac{1}{2}). \qquad [54]$$

The spin angle functions defined in Eq. (51) are eigenfunctions of J^2, J_z, and L^2, where J is the total angular momentum $\vec{J} = \vec{L} + \vec{S}$ · μ now refers to the projection quantum number $\mu = J_z = 1_z + s_z = m + m_s$. The χ_κ^μ are also eigenfunctions of the spin-orbit coupling operator introduced by Dirac (in units of h = c = 1)

$$(\vec{\sigma}\cdot\vec{L} + 1)\, \chi_\kappa^\mu = -\kappa\, \chi_\kappa^\mu \qquad [55]$$

Since $-\kappa$ and $1_{(-\kappa)}$ are defined, it is easy to introduce $\chi_{-\kappa}^\mu$ as follows

$$\chi_{-\kappa}^{\mu} = \sum_{\tau = \pm\frac{1}{2}} C_{\mu-\tau\ \ \tau\ \ \mu}^{\ell(-\kappa)\ \ \frac{1}{2}\ \ |\kappa|-\frac{1}{2}} \, Y_{\ell(-\kappa)}^{\mu-\tau} \, \chi_{\frac{1}{2}}^{\tau} \qquad [56]$$

The operator that connects the two spin-angle functions is

$$\frac{\vec{\sigma}\cdot\vec{r}}{r} \equiv \vec{\sigma}\cdot\hat{r} \qquad [57]$$

and the connecting relationship is

$$\vec{\sigma}\cdot\hat{r}\,\chi_{\kappa}^{\mu} \equiv \left(\frac{\vec{\sigma}\cdot\vec{r}}{r}\right)\chi_{\kappa}^{\mu} = -\chi_{-\kappa}^{\mu} \qquad [58]$$

The explicit form of the spin-angle functions in all four important cases is given below.

For the case $j = \ell - \frac{1}{2}$ $(\kappa > 0)$, $\kappa = \ell$ and $\bar{\ell} = \ell - 1$

$$\chi_{\kappa}^{\mu} = \begin{pmatrix} -\sqrt{\frac{\ell-\mu+\frac{1}{2}}{2\ell+1}} \; Y_{\ell}^{\mu-\frac{1}{2}} \\ \sqrt{\frac{\ell+\mu+\frac{1}{2}}{2\ell+\frac{1}{2}}} \; Y_{\ell}^{\mu+\frac{1}{2}} \end{pmatrix} \qquad [59a]$$

and

$$\chi_{-\kappa}^{\mu} = \begin{pmatrix} \sqrt{\frac{\ell+\mu-\frac{1}{2}}{2\ell-1}} \; Y_{\ell-1}^{\mu-\frac{1}{2}} \\ \sqrt{\frac{\ell-\mu-\frac{1}{2}}{2\ell-1}} \; Y_{\ell-1}^{\mu+\frac{1}{2}} \end{pmatrix} \qquad [59b]$$

For the opposite case, where $j = \ell + \frac{1}{2}$ $(\kappa < 0)$, $\kappa = -\ell - 1$ and $\bar{\ell} = \ell + 1$

$$\chi_{\kappa}^{\mu} = \begin{pmatrix} \sqrt{\dfrac{\ell+\mu+\frac{1}{2}}{2\ell+1}} \; Y_{\ell}^{\mu-\frac{1}{2}} \\ \sqrt{\dfrac{\ell-\mu+\frac{1}{2}}{2\ell+1}} \; Y_{\ell}^{\mu+\frac{1}{2}} \end{pmatrix} \qquad [59c]$$

and

$$\chi_{-\kappa}^{\mu} = \begin{pmatrix} -\sqrt{\dfrac{\ell-\mu+\frac{3}{2}}{2\ell+3}} \; Y_{\ell+1}^{\mu-\frac{1}{2}} \\ \sqrt{\dfrac{\ell+\mu+\frac{3}{2}}{2\ell+3}} \; Y_{\ell+1}^{\mu+\frac{1}{2}} \end{pmatrix} \qquad [59d]$$

The spin angle functions form an orthonormal set in spin-angle space

$$\langle \chi_{\kappa'}^{\mu'} | \chi_{\kappa}^{\mu} \rangle = \delta_{\kappa\kappa'} \delta_{\mu\mu'} \qquad [60]$$

where the scalar product implies integration over the angles and summation over the spin indices.

Since multiplication of these spin-angle functions by any function of r does not alter the angular properties of these functions, in particular their relationship to J^2, L^2, J_z, $\vec{\sigma}\cdot\vec{L} + 1$ and $\vec{\sigma}\cdot\hat{r}$, we can introduce the spinors

$$|v\ \kappa\ \mu> \rightarrow \chi_{\kappa}^{\mu}\ F_{v\ell} \qquad [61a]$$

$$|v\ -\kappa\ \mu> \rightarrow i\ \chi_{-\kappa}^{\mu}\ F_{v\bar{\ell}} \qquad [61b]$$

Here $F_{vl}(r)$ is the normalized radial solution of the non-relativistic isotropic harmonic oscillator

$$F_{v\ell}(r) = \left\{ \frac{2\lambda^3\ \Gamma(v+\ell+\frac{3}{2})}{v!\,[\Gamma(\ell+\frac{3}{2})]^2} \right\}^{\frac{1}{2}} (\lambda r)^{\ell}\, e^{-\frac{1}{2}\lambda^2 r^2}\ {}_1F_1\left(\begin{matrix} -v \\ \ell+\frac{3}{2} \end{matrix} ; \lambda^2 r^2 \right) \qquad [62]$$

Now the orthonormal property of these spinors can be generalized

$$\langle v'\kappa'\mu' | v\kappa\mu \rangle = \delta_{vv'} \delta_{\kappa\kappa'} \delta_{\mu\mu'} \qquad [63]$$

v is the quantum number which, with 1, determines the oscillator energy levels

$$E_{vl} = (2v + 1 + 3/2) \hbar\omega \qquad [64]$$

The EHO is obtained by adding the interaction

$$V = i \lambda^2 \rho_1 (\vec{\sigma}\cdot\vec{r}) \frac{\vec{\sigma}\cdot\vec{L} + 1}{|\vec{\sigma}\cdot\vec{L} + 1|} \qquad [65]$$

to the free particle Dirac Hamiltonian (units of $\hbar = c = 1$)

$$H_{fp} = \rho_3 (m_o) + \rho_1 (\vec{\sigma}\cdot\vec{P}) \qquad [66]$$

This has exact eigenvalues and eigenfunctions as follows:

$$H \Psi_{v\kappa\mu} = E \Psi_{v\kappa\mu} \qquad [67a]$$

$$E = \sqrt{m_o^2 + 4\lambda^2 (v + |\kappa| + \tfrac{1}{2})} \qquad [67b]$$

In terms of the spinors given in Eq. (59) the above solutions $\Psi_{v\kappa\mu}$ are given explicitly by

$$\Psi_{v\kappa\mu} = \left\{ 1 + \frac{(E - m_o)^2}{4\lambda^2 (v + |\kappa| + \frac{1}{2})} \right\}^{-\frac{1}{2}} \begin{pmatrix} |v\ \kappa\ \mu\rangle \\ \dfrac{S_\kappa (E - m_o)}{2\lambda\sqrt{v + |\kappa| + \frac{1}{2}}} \ |v\ {-\kappa}\ \mu\rangle \end{pmatrix} \qquad [68]$$

and the bound state normalized constant is

$$\left[1 + \frac{(E - m_o)^2}{4\lambda^2 (v + |\kappa| + \frac{1}{2})}\right]^{-\frac{1}{2}} \qquad [69]$$

Explicit forms of the solutions fro the two cases of importance $j = \ell + \frac{1}{2}$ and $j = \ell - \frac{1}{2}$ are given below for $j = \ell + \frac{1}{2}$ $(\kappa < 0)$

$$\Psi_{\nu\kappa\mu} = \left\{ 1 + \frac{(E-m_0)^2}{4\lambda^2(\nu+|\kappa|+\frac{1}{2})} \right\}^{-\frac{1}{2}} \begin{bmatrix} \sqrt{\frac{\ell+\mu+\frac{1}{2}}{2\ell+1}} \; F_{\nu\ell} \, Y_{\ell}^{\mu-\frac{1}{2}} \\ \sqrt{\frac{\ell-\mu+\frac{1}{2}}{2\ell+1}} \; F_{\nu\ell} \, Y_{\ell}^{\mu+\frac{1}{2}} \\ \frac{i(E-m_0)}{2\lambda\sqrt{\nu+|\kappa|+\frac{1}{2}}} \sqrt{\frac{\ell-\mu+\frac{3}{2}}{2\ell+3}} \; F_{\nu\ell+1} \, Y_{\ell+1}^{\mu-\frac{1}{2}} \\ \frac{-i(E-m_0)}{2\lambda\sqrt{\nu+|\kappa|+\frac{1}{2}}} \sqrt{\frac{\ell+\mu+\frac{3}{2}}{2\ell+3}} \; F_{\nu\ell+1} \, Y_{\ell+1}^{\mu+\frac{1}{2}} \end{bmatrix} \qquad [70a]$$

for $j = \ell - \frac{1}{2}$ $(\kappa > 0)$

$$\Psi_{\nu\kappa\mu} = \left\{ 1 + \frac{(E-m_0)^2}{4\lambda^2(\nu+|\kappa|+\frac{1}{2})} \right\}^{-\frac{1}{2}} \begin{bmatrix} -\sqrt{\frac{\ell-\mu+\frac{1}{2}}{2\ell+1}} \; F_{\nu\ell} \, Y_{\ell}^{\mu-\frac{1}{2}} \\ \sqrt{\frac{\ell+\mu+\frac{1}{2}}{2\ell+1}} \; F_{\nu\ell} \, Y_{\ell}^{\mu+\frac{1}{2}} \\ \frac{i(E-m_0)}{2\lambda\sqrt{\nu+|\kappa|+\frac{1}{2}}} \sqrt{\frac{\ell+\mu-\frac{1}{2}}{2\ell-1}} \; F_{\nu\ell-1} \, Y_{\ell-1}^{\mu-\frac{1}{2}} \\ \frac{i(E-m_0)}{2\lambda\sqrt{\nu+|\kappa|+\frac{1}{2}}} \sqrt{\frac{\ell-\mu-\frac{1}{2}}{2\ell-1}} \; F_{\nu\ell-1} \, Y_{\ell-1}^{\mu+\frac{1}{2}} \end{bmatrix} \qquad [70b]$$

As was shown in ref. 14, in the non-relativistic limit, the EHO Hamiltonian yields the usual isotropic harmonic oscillator Hamiltonian with a spin-orbit coupling term of the Thomas-Frenkel form.

$$H_{NR} = \left(1 + \frac{3}{2}\lambda^2 S_x\right) m_0 + \frac{P^2}{2m_0} + \frac{\lambda^4}{2m_0} r^2 + \left(\frac{\lambda^2}{m_0} S_x\right) \vec{\sigma} \cdot \vec{L} \qquad [71]$$

The degeneracy of the energy levels of EHO is four times that of the non-relativistic oscillator and a comparison of these degeneracies is given in Table I.

TABLE I

DEGENERACY OF THE EHO AND THE NRHO

EHO			NRHO		
$E^2 - m_o^2 c^4$	$v + \lvert\kappa\rvert$	Degeneracy	E	$2v + \ell$	Degeneracy
$6\lambda^2$	1	4	$\frac{3}{2}\hbar\omega$	0	1
$10\lambda^2$	2	12	$\frac{5}{2}\hbar\omega$	1	3
$14\lambda^2$	3	24	$\frac{7}{2}\hbar\omega$	2	6
$18\lambda^2$	4	40	$\frac{9}{2}\hbar\omega$	3	10
$22\lambda^2$	5	60	$\frac{11}{2}\hbar\omega$	4	15
$26\lambda^2$	6	84	$\frac{13}{2}\hbar\omega$	5	21

CHAPTER IV

BREMSSTRAHLUNG WEIGHTED CROSS SECTION

The bremsstrahlung weighted cross section is defined as

$$\sigma_b = \int (\sigma/w)\, dw \qquad [72]$$

where σ_b is the electric dipole cross section for the nuclear photo-effect weighted by the dW/W approximation to the bremsstrahlung spectrum. σ_b is rather easily compared with measured bremsstrahlung yields for photonuclear processes. As has been shown by Levinger and Bethe(7) σ_b is not changed by the neutron-proton exchange force and, in the harmonic oscillator approximation, of the nuclear shell model, σ_b is proportional to the nuclear radius. For this reason sometimes the experiment is used as a means of determining the nuclear radius parameter r_o. Experimentally the total photonuclear cross section has been determined by measuring the attenuation of the photon flux from betatron gamma rays or some other copious source, using a Compton spectrometer with good resolution(12). The loss of intensity in the incident photon stream is partly due to nuclear absorption and partly due to electronic absorption. However, since accurate theoretical cross sections are available for photon-electron interactions such as the Compton effect, pair production, radiative corrections, it is possible to subtract the electronic absorption from the measured attenuation and get a fairly accurate value for the cross section due to nuclear absorption. This type of experiment is preferred to measuring the partial cross sections--ν-p, ν-n, ν-ν cross sections--and summing these because of the uncertainties concerning the geometry involved in the latter. While the nuclear part of the absorption is only a small fraction of the total loss of photons in the incident beam, in the case of light nuclei the nuclear part of the total cross section happens to be well distinguishable. Several experiments have been made on light closed-shell nuclei.

The cross section for a particle in an initial state $|0>$ to make a transition to another stationary state $|n>$ by photon absorption is obtained from the transition probability computed according to time dependent perturbation theory in quantum mechanics. According to the semiclassical theory of interaction of radiation with matter the photon is described by the vector potential

$$\vec{A} = \hat{z} A_o e^{-ikx} \qquad [73]$$

Here the gamma ray is assumed to be polarized along the Z axis and propagating along the x direction and the amplitude A_o determines the number of photons in the incident flux. In the nonrelativistic Schrodinger theory the Hamiltonian for an electron in a pure radiation field is given by the gauge invariant substitution

$$\vec{P} \to \vec{P} + \frac{e}{c}\vec{A} \quad , \quad E \to E + e\phi \qquad [74a]$$

Such that

$$\vec{P}^2 \to \vec{P}^2 + \frac{e}{c}\vec{P}\cdot\vec{A} + \frac{e}{c}\vec{A}\cdot\vec{P} + \frac{e^2}{c^2}\vec{A}^2 \qquad [74b]$$

and the Schrödinger equation becomes

$$[\frac{1}{2m}(\vec{P}^2 + \frac{e}{c}\vec{P}\cdot\vec{A} + \frac{e}{c}\vec{A}\cdot\vec{P} + \frac{e^2}{c^2}\vec{A}^2) + V]\ \Psi = E\Psi \qquad [75]$$

The term in $\vec{A}^2$ gives rise to second order transitions in which more than one photon is involved which is negligible and in the radiation gauge $\nabla\cdot\vec{A} = 0$, $\phi = 0$, the two terms $\frac{e}{2mc}(\vec{P}\cdot\vec{A} + \vec{A}\cdot\vec{P})$ combine to give the perburbing potential

$$\frac{e}{mc}\vec{A}\cdot\vec{P} = -\frac{ie\hbar}{mc}\vec{A}\cdot\vec{\nabla} \qquad [76]$$

The transition probability between states $|0\rangle$ and $|n\rangle$ is proportional to the absolute square of the matrix element

$$\langle 0|\ A_o e^{-ikx}\ \hat{z}\cdot\vec{\nabla}\ |n\rangle \qquad [77]$$

For photon energies of experimental interest and where the radiation is observed far away from the atom kx is very small compared to 1 and hence the exponential in the perturbing potential can be replaced by unity. This is known as the dipole approximation or neglect of the retardation factor. The time factor is eliminated by conservation of energy between the initial state of the particle $|0\rangle$, the final state of the particle $|n\rangle$ and the photon energy. The vector potential has, of course, to be real and this necessitates the addition of the complex conjugate to the term in Equation (77), however, this leads to emission of a gamma ray and hence can be set equal to zero in absorption probability calculations. Applying Heisenberg matrix mechanics and the Bohr frequency rule, the above matrix element can be related to the oscillator strength as the following steps show.

Since

$$\langle 0|\ \hat{z}\cdot\vec{\nabla}|n\rangle = \frac{i}{\hbar}\langle 0|\ P_z|n\rangle \qquad [78]$$

and

$$\frac{1}{m} \langle 0|P_z|n\rangle = \langle 0|\dot{z}|n\rangle = \frac{i}{\hbar}(E_n - E_o)\langle 0|z|n\rangle = i\,\omega_{on}\langle 0|z|n\rangle \qquad [79]$$

then the matrix element becomes, in the dipole approximation,

$$-\frac{m}{\hbar}\,\omega_{on}\,\langle 0|z|n\rangle. \qquad [80]$$

If we compare with the definition of the oscillator strengths, as given in Eq. (20), it is easy to see they are related by a constant (-2). The cross section for the absorption of a photon of energy $W = E_n - E_o$ is then given by[7]

$$\sigma_{on} = \frac{2\pi^2 e^2 \hbar}{\mu c} f_{on} = \frac{4\pi^2 e^2}{\hbar c}(E_n - E_o)|\langle 0|z|n\rangle|^2 \qquad [81]$$

From the above we get the bremsstrahlung weighted cross section for a one particle quantum mechanical system as

$$\begin{aligned} \sigma_b &= \int \left(\frac{\sigma_{on}}{W}\right) dW \\ &= \frac{4\pi^2 e^2}{\hbar c} \sum_n |\langle 0|z|n\rangle|^2 \qquad [82] \\ &= \frac{4\pi^2 e^2}{\hbar c} \langle 0|z^2|0\rangle \end{aligned}$$

In the above the closure property has been used in the summation over n. It is thus seen that the crux of the problem is to evaluate the ground state expectation value of the operator z^2 for the appropriate quantum mechanical system.

For a nuclear transition from the ground state $|0\rangle$ to any excited state $|n\rangle$ the wave functions of both the states have to be known. Rather little is known of the wave function of the ground state of the whole nucleus and much less of the excited state $|n\rangle$. It is therefore customary to work in some model of the nucleus and the one best suited to this problem is the well known shell model or the independent particle model. Bethe and Levinger[7] were the first to derive a formula for the bremsstrahlung weighted cross section for the nucleus, proceeding along the lines of the derivation given above for a one particle problem. If we consider the displacement from the center of mass of the nucleus, each proton behaves as if its charge were eN/A where N is the neutron number and, similarly, each neutron as if its charge were - eZ/A. For a many particle system the appropriate operator in the dipole approximation is $\sum_i Z_i$ where Z_i is the component of the displacement along the direction of polarization of the incident photon. Bethe and Levinger derived the following formula for the bremsstrahlung weighted cross section

$$\sigma_b = \int_0^\infty \left(\frac{\delta}{W}\right) dW$$

$$= \left(\frac{e^2}{\hbar c}\right) (4\pi^2) \langle 0| \left[\frac{N}{A} \sum_i Z_i - \frac{Z}{A} \sum_j Z_j\right]^2 |0\rangle \qquad [83]$$

In the above the suffix i refers to protons and the suffix j to neutrons, and the expectation value is taken with respect to the ground state wave function of the nucleus $|0\rangle$. The important consideration then is to know the ground state wave function as accurately as possible. Levinger and Bethe used the Fermi gas model and a Hartree type product many particle wave function with single particle plane wave functions as factors. Levinger[13] used a more realistic independent particle model. He chose the isotropic harmonic oscillator model and used a many particle wave function which was a product of two Slater determinants, one representing antisymmetrized proton states and the other antisymmetrized neutron states. In other words Levinger introduced positional correlations in the motions of protons and neutrons separately in accordance with the Pauli principle. He arrived at the remarkably simple formula for the bremsstrahlung weighted cross section

$$\sigma_b = 0.36 \; A^{4/3} \text{ mb} \qquad [84]$$

The above has been used ever since as the phenomenological or semiempirical formula for bremsstrahlung weighted cross section which, as seen above, depends only on the mass number of the absorbing nucleus or more appropriately the one parameter viz., the radius parameter which, in the harmonic oscillator approximation, can be fixed from the oscillator constant λ. The Pauli principle correlations decrease σ_b since due to the exclusion principle each proton is surrounded by an 'exchange hole' in which there is a decreased likelihood of finding another proton. The shell model, of course, ignores other dynamical correlations like the spin dependent force between nucleons--attractive forces in a mutual triplet spin state of two nucleons and repulsive in singlet states. While a detailed comparison of experiment and theory will be postponed to a later chapter, it is important to note that the simple Levinger formula is not in agreement with experiment in all cases and there has been need to look for corrections to this formula.

The simplest and most straightforward extension of Levinger's theory attempted in this work is to replace the non-relativistic isotropic harmonic oscillator by a relativistic oscillator model of the nucleus(8). As has been discussed in an earlier chapter, this EHO Hamiltonian has the merit of analytical simplicity as well as a physically significant non-relativistic limit; that of the isotropic oscillator with a spin orbit coupling of the Thomas-Frenkel form. The single particle states are then given by the spinor wave function $\Psi_{\nu\kappa\mu}$ of the earlier chapter and the ground state of the nucleus is described by the antisymmetrized (protons and neutrons separately) wave function made up of these single particle states in the usual way as a Slater determinant. This makes sure that positional correlations are included. This ground state wave function is used in Eq. (83) to compute the bremsstrahlung weighted cross section. The following equations summarize the formula one obtains when relativistic wave functions are used. They are naturally more complicated than the non-relativistic formulas but in the approximation v/c--0 the simple formula of Levinger is obtained.

$$\begin{aligned}\sigma_b &= \frac{4\pi^2 e^2}{\hbar c} \langle 0 | \left[\frac{N}{A}\sum_i z_i - \frac{Z}{A}\sum_j z_j\right]^2 | 0 \rangle \\ &= \frac{4\pi^2 e^2}{\hbar c}\Bigg\{\frac{N^2}{A^2}\langle 0|\sum_i z_i^2|0\rangle + \frac{N^2}{A^2}\langle 0|\sum_{\substack{i\ i' \\ i\neq i'}}\sum z_i z_{i'}|0\rangle \\ &\quad + \frac{Z^2}{A^2}\langle 0|\sum_j z_j^2|0\rangle + \frac{Z^2}{A^2}\langle 0|\sum_{\substack{j\ j' \\ j\neq j'}}\sum z_j z_{j'}|0\rangle \\ &\quad - \frac{2NZ}{A^2}\langle 0|\sum_i\sum_j z_i z_j|0\rangle\Bigg\}\end{aligned} \qquad [85]$$

where $i = 1, 2, 3, \ldots. Z$

$j = Z + 1, Z + 2, \ldots. Z + N$

and $|0\rangle$, the ground state wave function of nucleus when Pauli principle correlation is taken into account, can be expressed explicitly as follows:

$$|0\rangle = \frac{1}{\sqrt{N!}\sqrt{Z!}} \begin{vmatrix} \psi_{a_1}(\vec{r}_1) & \psi_{a_1}(\vec{r}_2) & \cdots & \psi_{a_1}(\vec{r}_Z) \\ \psi_{a_2}(\vec{r}_1) & \psi_{a_2}(\vec{r}_2) & \cdots & \psi_{a_2}(\vec{r}_Z) \\ \vdots & \vdots & & \vdots \\ \psi_{a_Z}(\vec{r}_1) & \psi_{a_Z}(\vec{r}_2) & \cdots & \psi_{a_Z}(\vec{r}_Z) \end{vmatrix} \begin{vmatrix} \psi_{a_1}(\vec{r}_{Z+1}) & \psi_{a_1}(\vec{r}_{Z+2}) & \cdots & \psi_{a_1}(\vec{r}_{Z+N}) \\ \psi_{a_2}(\vec{r}_{Z+1}) & \psi_{a_2}(\vec{r}_{Z+2}) & \cdots & \psi_{a_2}(\vec{r}_{Z+N}) \\ \vdots & \vdots & & \vdots \\ \psi_{a_N}(\vec{r}_{Z+1}) & \psi_{a_N}(\vec{r}_{Z+2}) & \cdots & \psi_{a_N}(\vec{r}_{Z+N}) \end{vmatrix} \qquad [86]$$

In the last equation $\Psi_{a_k}(\vec{\gamma}_i)$ is the normalized wave function $\Psi_{v\kappa\mu}$ of the i^{th} particle in the quantum state described by the quantum numbers u, κ, and μ [$\equiv a_k$], then, the results of the required matrix elements in Eq. (85) are obtained as follows, by using the orthogonal properties and the selection rules.

$$\langle 0|z_i^2|0\rangle = \frac{1}{Z}\sum_{\ell=1}^{Z} \langle \psi_{a_\ell}(\vec{r}_i)|\, z_i^2\, |\psi_{a_\ell}(\vec{r}_i)\rangle \qquad [87a]$$

$$\langle 0|z_j^2|0\rangle = \frac{1}{N}\sum_{\ell=1}^{N} \langle \psi_{a_\ell}(\vec{r}_j)|\, z_j^2\, |\psi_{a_\ell}(\vec{r}_j)\rangle \qquad [87b]$$

$$\langle 0|z_i z_{i'}|0\rangle = \frac{1}{Z(Z-1)} \sum_{\substack{\ell=1 \\ \ell\neq m}}^{Z}\sum_{m=1}^{Z} (-) \langle \psi_{a_\ell}(\vec{r}_i)|z_i|\psi_{a_m}(\vec{r}_i)\rangle$$
$$\times \langle \psi_{a_m}(\vec{r}_{i'})|z_{i'}|\psi_{a_\ell}(\vec{r}_{i'})\rangle \qquad [87c]$$

$$\langle 0|z_i z_{i'}|0\rangle = \frac{1}{N(N-1)} \sum_{\substack{l=1 \\ l\neq m}}^{N} \sum_{m=1}^{N} (-) \langle \psi_{a_l}(\vec{r}_i)|z_i|\psi_{a_m}(\vec{r}_i)\rangle$$
$$\times \langle \psi_{a_m}(\vec{r}_{i'})|z_{i'}|\psi_{a_l}(\vec{r}_{i'})\rangle \qquad [87d]$$

$$\langle 0|Z_i\ Z_j|0\rangle = 0 \qquad [87e]$$

Two questions arise in the application of the above formula to a particular nucleus for purposes of comparison with experimental results. Firstly the quantum numbers of the single particles outside closed shells have to be fixed. This becomes a problem if we remember that the multiplicities and degeneracies are not the same in the relativistic and non-relativistic models. However, since the Dirac angular momentum quantum number κ relates to j it is realistic to choose the appropriate quantum numbers in such a way that the experimentally known spin of the nucleus (j value) is reproduced. The appropriate quantum numbers of the outermost nucleon or nucleons in the cases studied are given in Table II. The second question is the choice of the one parameter in the oscillator model--whether relativistic or non-relativistic--viz., the oscillator constant λ. In the non-relativistic case the equivalent uniform radius of the nucleus in a linear function of the oscillator constant; as can be seen from the following equations:

$$\langle v l|r^2|v l\rangle = \frac{1}{\lambda^2}\left(2v + l + \frac{3}{2}\right) \qquad [88]$$

$$\langle r^2\rangle_{\text{nucleus}} = \frac{1}{\lambda^2}\left[\frac{1}{A}\sum_{v}\sum_{\lambda}\left(2v + l + \frac{3}{2}\right)(2l+1)\right] \qquad [89]$$

since,

$$R^2_{uniform} = \frac{5}{3} \langle r^2 \rangle_{nucleus} \qquad [90]$$

such that

$$R_{uniform} = \frac{1}{\lambda} \left[\frac{5}{3A} \sum_{v} \sum_{\ell} (2v+\ell+\tfrac{3}{2})(2\ell+1) \right] \qquad [91]$$

If, therefore, the uniform radius of the nucleus is chosen in accordance with the well known formula

$$R = r_o A^{1/3} \qquad [92]$$

then from Eq. (91), the oscillator constant is fixed depending on the choice of r_o. Levinger chose r_o = 1.2 fermis which was the best known value from other experimental studies of nuclear sizes, coulomb energies of mirror nuclei, mesonic x-rays, etc. This way of fixing the oscillator parameter is not applicable to the relativistic case easily. The energy of the state pertaining to the quantum numbers enters the wave function implicitly and this leads to a transcendental equation for λ in the expression for the uniform radius. It has been noticed, however, that the error involved in accepting the non-relativistic value is negligible.

The nuclei chosen for study lie in the regions of light nuclei, intermediate nuclei and very heavy nuclei. Calculations have been made for representative nuclei for which both experimental data and non-relativistic estimates exist. Detailed comparison of the relativistic results with experiment is given in the concluding chapter. Because of the complicated nature of the formula (85), the cross sections had to be numerically evaluated. The relevant computer program is appended.

TABLE II

THE QUANTUM NUMBERS OF THE OUTERMOST NUCLEONS OUTSIDE CLOSED SHELLS

Nuclides	Ordinal No. of Nucleon	v	κ	μ
$^{12}_{6}C$	5	0	-2	$+\frac{1}{2}$
	6	0	-2	$-\frac{1}{2}$
$^{19}_{9}F$	9	1	-1	$+\frac{1}{2}$
	10	1	-1	$-\frac{1}{2}$
$^{98}_{42}Mo$	41	0	-4	$+\frac{1}{2}$
	42	0	-4	$-\frac{1}{2}$
$^{208}_{82}Pb$	81	0	-5	$+\frac{1}{2}$
	82	0	-5	$-\frac{1}{2}$
	123	2	+3	$+\frac{1}{2}$
	124	2	+3	$-\frac{1}{2}$
	125	2	+3	$+\frac{3}{2}$
	126	2	+3	$-\frac{3}{2}$

CHAPTER V

RELATIVISTIC OSCILLATOR STRENGTHS

The definition and calculation of oscillator strengths in the earlier chapter are based on the non-relativistic Schrödinger equation for central fields. The interaction between the charged particle e and the radiation field (not quantized) is taken, in the radiation gauge, to be

$$\frac{ie\hbar}{mc} \vec{A}\cdot\vec{\nabla} \qquad [93]$$

Here $\vec{A}$ is the vector potential which, in the cases of emission and absorption of radiation accompanied by transition between stationary states, is expressed as

$$\vec{A} = A_o \, \hat{e} \, e^{\pm i \, \vec{k}\cdot\vec{r}} \qquad [94]$$

where $\hat{e}$ is the unit vector in the direction of polarization of a linearly polarized electromagnetic wave. From the above two equations one eventually introduces the oscillator strength as

$$f_{n'n} = \frac{2m}{\hbar} \omega_{n'n} \, |\langle n'|z|n\rangle|^2 \qquad [95a]$$

or

$$f_{n'n} = \frac{2}{\hbar m \, \omega_{n'n}} \, |\langle n|P_z|n'\rangle| \, |\langle n'|P_z|n\rangle| \qquad [95b]$$

It is the second expression which contains matrix elements of the momentum operator between the appropriate stationary state wavefunctions of the charged particle interacting with radiation, that makes transition to relativistic theory convenient. It is well known that for an adequate description of the processes of absorption, spontaneous and induced emission of radiation by matter consistent with experimental facts, it is necessary to quantize the electromagnetic field as well. In this theory also the basic interaction of the charged particle with the electromagnetic field, which is treated as a perturbation, is given by

$$-\frac{e}{mc}\vec{A}\cdot\vec{P} \qquad [96]$$

In the dipole approximation, or neglecting the retardation factor $e^{i\vec{k}\cdot\vec{r}}$, the oscillator strength is still given by Eq. (95). The justification for this may be in the fully relativistic and quantized derivation of the Kramers Heisenberg Dispersion theory(5) from which the oscillator strength can be extracted just as in the non-relativistic theory. Payne and Levinger(11) calculated the relativistic oscillator strengths both in the dipole approximation and in a more exact formulation including the retardation factors, for the Dirac-Coulomb case. In other words, in their calculations, the basis states of the charged particle are the solutions of the Dirac equation with the Coulomb potential. Jacobsohn (15) gave relativistic oscillator strengths for dipole transitions from the L shell. Massey and Burhop(16) calculated the relativistic non-retarded transition rate of K x-rays of $_{79}$Au. While all these have been numerical calculations in the main, through an entirely different approach Gell-mann, Goldberger and Thirring derived the sum rule for dipole transitions by considering the dispersion relation obeyed by the forward scattering amplitude of a bound electron scattering a high energy photon. While their derivation agreed with the familiar Thomas-Reiche-Kuhn sum rule, Levinger's calculation disagreed with this conclusion and showed that the scattering by a free electron and a bound electron of a high energy photon cannot be considered to be equal.

It is easy to see that the derivation of the sum rule made in the non-relativistic theory cannot be duplicated in the relativistic theory. For instance, the starting point in the non-relativistic derivation was the double commutator

$$[[H,Z],Z] \qquad [97]$$

the expectation value of which in the basis of a complete set of states led to the sum rule. If we replace the non-relativistic central field Hamiltonian

$$H_{nr} = \frac{1}{2m}\vec{P}^2 + V(r) \qquad [98]$$

by the Dirac Hamiltonian

$$H = \rho_3 m_o + \rho_1 \vec{\sigma}\cdot\vec{P} + V(r) \qquad [99]$$

the double commutator vanishes as follows:

$$[H,Z] = [\rho_1 \vec{\sigma}\cdot\vec{P}, Z] = -i\rho_1\sigma_z \qquad [100a]$$

$$[[H, Z], Z] = 0 \qquad [100b]$$

since $$[\rho_i, Z] = [\sigma_i, Z] = 0 \qquad [100c]$$

This happens because of the basic difference in the dynamical description of the momentum of a particle in the two theories. In the non-relativistic theory the momentum operator follow the Schrodinger prescription $\vec{P} = -i\hbar\vec{\nabla}$ whereas in the relativistic theory the momentum operator is given by

$$\vec{P} = m_o c \, \vec{\alpha} \qquad [101]$$

and correspondingly the oscillator strength is given by the expression

$$f_{n'n} = \frac{2m_o c^2}{\hbar \, \omega_{n'n}} \, |\langle n'|\alpha_z|n\rangle|^2 \qquad [102]$$

This basic difference can also perhaps be related to the well known phenomenon wherein the position operator in Dirac theory does not exactly correspond to the position operator in the Schrodinger theory inasmuch as the particle can be localized only within an error in measurement corresponding to the Compton wavelength of the particle. Incidentally it is interesting to note that the above double commutator does not vanish in the EHO case because the operator z does not commute with the EHO potential

$$[z, \; i\lambda^2 \rho_1 (\vec{\sigma}\cdot\vec{r}) \, \frac{\vec{\sigma}\cdot\vec{L} + 1}{|\vec{\sigma}\cdot\vec{L} + 1|}] \neq 0 \qquad [103]$$

whereas z does commute with the Coulomb potential e^2/r. It is, therefore, necessary to compute the oscillator strengths and the sum rule numerically starting from the basic matrix element

$$\langle n'|\vec{\alpha}|n\rangle \qquad [104]$$

using as basis functions the solutions of the EHO $\Psi_{\nu\kappa\mu}$. While the numerical results are presented and discussed in the next chapter, there is one other point to note. Usually the experiment does not distinguish between the three mutually perpendicular directions along which the photon may be linearly polarized. The oscillator strengths should, therefore, be averaged over the photon polarizations. Furthermore in all central fields, relativistic or non-relativistic, the chosen initial state described by a given set of quantum numbers is usually degenerate in energy. Since different sets of quantum numbers describing the initial state can have the same energy, in the sum rule calculations it will be meaningful if a further averaging is done over the different degenerate initial states. This question is not crucial in the non-relativistic case of a one particle system because, as Bethe and Salpeter(17) have shown, once the sum over photon polarizations is made, the result happens to be independent of the magnetic quantum number m because of the selection rules. Similarly the sum over m makes the result independent of the orbital angular quantum number ℓ and thus it is immaterial whether or not this averaging over initial states is done because the sum over final states and average over photon polarizations makes the result independent of the quantum numbers of the initial state. Some of the calculations of Bethe and Salpeter are reproduced here below. Unfortunately this is not the case for relativistic radiative transitions and this necessitates averaging over the degenerate initial states.

For a given v', the average oscillator strengths $\bar{f}_{n'n}$ is

$$\bar{f}_{n'n} = \frac{1}{3}\left\{ \frac{2m}{\hbar}\,\omega_{v\ell,v'\ell+1} \sum_i \sum_{m'} \left| \langle v\ell m | x_i | v'\ell+1\, m' \rangle \right|^2 + \frac{2m}{\hbar}\,\omega_{v\ell,v'\ell-1} \sum_i \sum_{m'} \left| \langle v\ell m | x_i | v'\ell-1\, m' \rangle \right|^2 \right\} \qquad [105a]$$

$$= \frac{1}{3}\left\{ \frac{2m}{\hbar}\omega_{v\ell,v'\ell+1}\left(\frac{\ell+1}{2\ell+1}\right)\left|\langle v\ell|r|v'\ell+1\rangle\right|^2 + \frac{2m}{\hbar}\omega_{v\ell,v'\ell-1}\left(\frac{\ell}{2\ell+1}\right)\left|\langle v\ell|r|v'\ell-1\rangle\right|^2 \right\}$$

[105b]

When summed over v' the sum rule for the average oscillator strengths is obtained as follows:

$$\sum_{n'} \bar{f}_{n'n} = \frac{2m}{3\hbar}\left(\frac{\ell+1}{2\ell+1}\right)\sum_{v'}\omega_{v\ell,v'\ell+1}\left|\langle v\ell|r|v'\ell+1\rangle\right|^2 + \frac{2m}{3\hbar}\left(\frac{\ell}{2\ell+1}\right)\sum_{v'}\omega_{v\ell,v'\ell-1}\left|\langle v\ell|r|v'\ell-1\rangle\right|^2$$

$$= \frac{1}{3}\,\frac{(\ell+1)(2\ell+3)}{(2\ell+1)} - \frac{1}{3}\,\frac{\ell(2\ell-1)}{(2\ell+1)}$$

$$= 1$$

[105c]

As in the non-relativistic case, when the sum is broken up into two different summations, one corresponding to higher energy of the final state (absorption) and another corresponding to lower energy (emission), absorption probability predominates over emission probability. In other words the jumps corresponding to absorption make a larger contribution to the summed oscillator strengths than the ones corresponding to emission. As will be seen later, the end result happens to be an agreement with Levinger and Payne's conclusion even in the nuclear case rather than with the Gell-mann, Goldberger, and Thirring's theorem.

CHAPTER VI

RESULTS AND CONCLUSIONS

As mentioned in the previous chapter, for the relativistic case the oscillator strengths and the sum rule had to be evaluated numerically. However, since the Pauli spinors χ_κ^μ in the solutions $\Psi_{v\kappa\mu}$ of the EHO are built out of the solutions of the non-relativistic Schrödinger equation for the isotropic harmonic oscillator, the calculations are considerably simplified because of selection rules resulting from the orthogonality of the spherical harmonics as well as the radial functions.

$$\langle \ell m | \ell' m' \rangle = \delta_{\ell\ell'} \delta_{mm'} \qquad [106a]$$

$$\langle v \ell | v' \ell \rangle = \delta_{vv'} \qquad [106b]$$

The final formula for the summed oscillator strengths becomes

$$\sum_{n'} f_{n'n} = \frac{1}{3} 2m_o c^2 \sum_{v'} \sum_{\kappa'} \sum_{\mu'} \sum_{i} \frac{1}{E_{v'\kappa'} - E_{v\kappa}} \left| \langle v'\kappa'\mu' | \alpha_i | v\kappa\mu \rangle \right|^2 \qquad [107]$$

where there is a further averaging over all the degenerate states represented by the quantum numbers v, κ and μ; v + $|\kappa|$ being constant. In the actual calculation the state chosen has the following quantum numbers and energy

$$v = o, \ |\kappa| = 3 \ \text{ or } \ v = 1, \ |\kappa| = 2 \ \text{ or } \ v = 2, \ |\kappa| = 1 \qquad [108]$$

and $$E_n = \sqrt{m_o^2 + 14\lambda^2}$$

There is an interesting point of difference between the matrix elements in the non-relativistic case and in the relativistic theory. In the radial integrals, arising from the basic operator α_i, one gets the radial matrix element

$$<v\ell|r|v'\ \ell'>$$

where $\ell' = \ell + 1$ or $\ell - 1$

whereas in the relativistic case, because of the operator α_i, one gets the overlap integral

$$<v\kappa\mu|v'\ -\kappa'\ \mu'> \;=\; \delta_{v\kappa'}\ \delta_{\kappa,-\kappa'}\ \delta_{\mu\mu'} \qquad [109]$$

and this introduces the selection rule $v' = v$, which simplifies the results considerably and reduces the total number of final discrete states to which transitions are probable. Since the calculations are done numerically it is necessary to choose one particular nucleus and the one chosen is $^{63}_{29}Cu$. The oscillator parameter λ is fixed by adjusting the radius of the equivalent uniform sphere to $r_o\ A^{1/3}$ fermis where r_o has been chosen as 1.2. This choice of the radius constant facilitates comparisons with the non-relativistic cases. The maximum number of final states to which a dipole transition is probable from the initial state $|0, -3, \tfrac{1}{2}>$ happens to be 7. Using the formula in Eq. 107 and averaging over the three directions of photon polarization as also the different degenerate states belonging to the energy level $v + |\kappa| = 3$, the numerical value of the sum is 0.94 and thus slightly departs from the non-relativistic value of 1. It is, of course, to be noted that the sum rule corresponds to the transitions of the 29th particle in that particular initial state, or stated more precisely, this sum rule is that of one particle in a given initial state described by the quantum numbers $v = o$, $\kappa = -3$ and $\mu = \frac{1}{2}$. The percentage departure from the non-relativistic value is linked with the approximate procedure used in fixing the oscillator parameter λ. In Chapter II the sum rule was evaluated in a more approximate way. Bethe's non-relativistic derivation was changed to the extent of calculating the matrix elements of z in the basis set $\Psi_{v\kappa\mu}$ in place of the solutions of the isotropic harmonic oscillator $U_{v\ell m}$ as the basis functions. The numerical value of the sum for the initial state $|0, -3\ \frac{1}{2}\rangle$ for the nucleus $A = 63$ turns out to be 0.91. This exhibits the unsatisfactory nature of the approximation in the evaluation of the sum rule by this semi-relativistic method.

For the nuclei of experimental interest ${}_2He^4$, ${}_6C^{12}$, ${}_8O^{16}$, ${}_9F^{19}$, ${}_{20}Ca^{40}$, ${}_{42}Mo^{98}$, ${}_{82}Pb^{208}$, calculations of the bremsstrahlung weighted cross section σ_b have been made using formula (85) in Chapter IV. As usual the one adjustable parameter λ has been chosen, following Levinger, such that the radius of the nucleus is equal to $r_o\ A^{1/3}$ fermis. The effect of different choices of r_o, which is a matter of dispute in the literature, has also been studied. The results are summarized in Tables III, IV and V. Several comparisons have to be made. There is the comparison of the overall result with the simple formula derived by Levinger[13]

$$\sigma_b = 0.36\ A^{4/3} \qquad [110]$$

and then there is the comparison with the calculations made using non-relativistic wave functions. To facilitate the latter comparison the following percentage is shown in Table III:

$$\frac{\text{Relativistic} - \text{nonrelativistic}}{\text{nonrelativistic}} \times 100$$

Tables IV and V emphasize that the above simple Levinger's phenomenological formula is not strictly correct. The constant .355 does not turn out to be a nucleus-independent constant but happens to be a function of the mass number A. However it is very interesting to note that a simple modification of Levinger's formula can be proposed

$$\sigma_b = 0.355 \left(\frac{r_o}{1.45}\right)^2 A^{1/3} (A + \Delta) \qquad [111]$$

where Δ is the correction factor which is shown in Table V. This correction factor is itself dependent on A and is slightly sensitive to the choice of r_o. It may not be too wrong to say, however, that averaging over all values of r_o the correction factor can be taken to be .025A and if this is substituted in Eq. (111) we can rewrite Levinger's fromula with a modified multiplying constant

$$\sigma_b = 0.364 \left(\frac{r_o}{1.45}\right) A^{4/3} \qquad [112]$$

Unfortunately the comparison with experiment is not very straightforward because the experimental results themselves have appreciable uncertainties in the measured cross section, as shown in Table III. It is not unreasonable to assert, however, that the relativistic values with the choice of r_o = 1.1 appear to fit experimental results better than the non-relativistic calculations and are decidedly superior to Levinger's simple formula. The latter formula, though based on the non-relativistic harmonic oscillator model, uses the approximation N = Z and hence checks with our calculations for these types of nuclei. The pronounced disagreement of Levinger's formula with experiment happens to be in the case of lead where the relativistic calculations with a smaller radius constant show very good agreement. It is quite probable, as has been shown by Braun, that in such a heavy nucleus with such tight packing of nucleons there may exist relativistic motions. To some extent this can also be said of a very light nucleus like helium where probably the nucleons almost simulate the motions of free particles. There is probably noticeable disagreement in the case of oxygen between theory and experiment and this is perhaps due to the existence of other modes in particular, the giant resonance which this kind of a theory cannot take into account.

In conclusion it appears to be safe to say that the dipole oscillator strengths' sum rule is not applicable, at least without suitable modifications, to relativistic quantum mechanical systems. There is strong ground for suspecting relativistic motions in helium and lead to the extent that photonuclear reactions and the bremsstrahlung weighted cross section can be accepted as representative experiments for nuclear structure. The simple formula of Levinger needs the slight modification suggested above.

TABLE III

BREMSSTRALUNG WEIGHTED CROSS SECTION σ_b IN UNITS OF 10^{-27} cm^2

Nucleus	Non-Relativistic			Relativistic						Levinger's Results	Experimental Results
	r_o = 1.1	r_o = 1.2	r_o = 1.3	r_o = 1.1	(%)	r_o = 1.2	(%)	r_o = 1.3	(%)		
${}^{4}_{2}He$	1.882	2.240	2.629	1.937	2.900	2.296	2.500	2.660	1.200	2.287	1.5 - 3.0
${}^{12}_{6}C$	8.143	9.690	11.373	8.414	3.333	9.968	2.867	11.657	2.500	9.893	5.4 - 12.0
${}^{16}_{8}O$	11.949	14.221	16.689	12.278	2.750	14.459	1.675	17.036	2.075	14.460	7.2 - 7.4
${}^{19}_{9}F$	14.985	17.833	20.929	15.455	3.142	18.313	2.692	21.420	2.347	18.262	11.4 - 16.8
${}^{40}_{20}Ca$	40.543	48.249	56.626	41.881	3.300	49.600	2.800	57.985	2.400	49.213	26 - 32
${}^{98}_{42}Mo$	131.170	156.103	183.204	135.175	3.053	160.190	2.618	187.365	2.271	161.668	110 - 140
${}^{208}_{82}Pb$	348.831	415.137	487.210	358.202	2.686	424.702	2.304	496.244	1.854	443.455	270 - 375

TABLE IV

$\delta_b / A^{4/3}$

Nucleus	Non-Relativistic			Relativistic			Levinger's Results
	$r_o = 1.1$	$r_o = 1.2$	$r_o = 1.3$	$r_o = 1.1$	$r_o = 1.2$	$r_o = 1.3$	
${}^{4}_{2}He$	0.296	0.353	0.414	0.305	0.362	0.419	0.36
${}^{12}_{6}C$	0.296	0.353	0.414	0.306	0.363	0.424	0.36
${}^{16}_{8}O$	0.296	0.353	0.414	0.305	0.359	0.423	0.36
${}^{19}_{9}F$	0.296	0.352	0.413	0.305	0.361	0.422	0.36
${}^{40}_{20}Ca$	0.296	0.353	0.414	0.306	0.363	0.424	0.36
${}^{98}_{42}Mo$	0.290	0.345	0.405	0.299	0.355	0.415	0.36
${}^{208}_{82}Pb$	0.283	0.337	0.395	0.291	0.345	0.403	0.36

TABLE V

VALUE OF THE CORRECTION FACTOR Δ IN RELATIVISTIC AND NON-RELATIVISTIC CASES

Nucleus	Non-Relativistic			Relativistic		
	Δ (r_o = 1.1)	Δ (r_o = 1.2)	Δ (r_o = 1.3)	Δ (r_o = 1.1)	Δ (r_o = 1.2)	Δ (r_o = 1.3)
$^{4}_{2}He$	0.000	0.000	0.000	0.116	0.100	0.048
$^{12}_{6}C$	0.000	0.000	0.000	0.400	0.344	0.300
$^{16}_{8}O$	0.000	0.000	0.000	0.440	0.268	0.332
$^{19}_{9}F$	-0.053	-0.053	-0.053	0.543	0.458	0.392
$^{40}_{20}Ca$	0.000	0.000	0.000	1.320	1.120	0.960
$^{98}_{42}Mo$	-2.000	-2.000	-2.000	0.931	0.514	0.180
$^{208}_{82}Pb$	-9.337	-9.337	-9.337	-4.000	-4.760	-5.653

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APPENDIX A

PROGRAM FOR THE REQUIRED MATRIX ELEMENTS IN THE CALCULATION OF σ_b WHEN NEHO MODEL IS USED

This program, written in the FORTRAN IV language, will print out the required matrix elements of σ_b in Eq. (85) of Chapter IV when the wave functions of NRHO model is used in $|0\rangle$. The oscillator constant λ is not included in this program.

$$\text{ZSQWO} = \langle 0|z_i{}^2|0\rangle$$

$$\text{ZIJWO} = \langle 0|z_i z_{i'}|0\rangle$$

The value of the variable N, is the number of protons in this program which must be changed for different nuclei. The input data are the quantum numbers v, ℓ, and m of the protons. Making use of Eq. (85) and the printed results the value of the bremsstrahlung weighted cross section σ_b can be calculated.

```
000000000111111111122222222223333333333444444444455555555556666666666777777777778
123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
CARD
$JOB
  101 FORMAT (4F5.1)
  102 FORMAT(1X,I5,5X,4F10.1,5X,E11.4,F10.4)
  103 FORMAT(1X,13HSUM OF ZSQVLM,5X,E11.4)
  104 FORMAT(1X,8HZSQWO IS,5X,E11.4)
  105 FORMAT(1X,2I5,10X,4E20.4)
  106 FORMAT(1X,8HZIJWO IS,5X,E11.4)
  107 FORMAT(1X,14HSUM OF ZIZJ IS,E11.4)
      S1(R1,R2)=SQRT(R1+R2+1.0/2.0)
      S2(R3)=SQRT(R3+1.0)
      S3(R4,R5)=SQRT(R4+R5+3.0/2.0)
      S4(R6,R7)=SQRT((R6*R6-R7*R7)/((2.0*R6+1.0)*(2.0*R6-1.0)))
      S5(R8,R9)=SQRT(((R8+1.0)*(R8+1.0)-R9*R9)/((2.0*R8+3.0)*(2.0*R8+1.0
     C)))
      REAL IV(130),IL(130),IM(130),IMS(130),ZSQVLM(130)
      SUM=0.0
      N=9
      ALPHA=1.0
      DO 10 I=1,N
      READ(5,101)IV(I),IL(I),IM(I),IMS(I)
      ZSQVLM(I)=(-1.0/ALPHA*ALPHA)*(2.0*IV(I)+IL(I)+3.0/2.0)*(1.0/3.0)*(
     C(2.0*(3.0*IM(I)*IM(I)-IL(I)*(IL(I)+1.0)))/((2.0*IL(I)-1.0)*(2.0*IL
     C(I)+3.0))-1.0)
      SUM=SUM+ZSQVLM(I)
      WRITE(6,102)I,IV(I),IL(I),IM(I),IMS(I),ZSQVLM(I) ,SUM
   10 CONTINUE
      WRITE(6,103)SUM
      ZSQWO=SUM/N
      WRITE(6,104)ZSQWO
      SUMM=0.0
      DO 20 L=1,N
      DO 20 K=1,N
      IF(L.EQ.K) GO TO 99
      IF(IMS(L)-IMS(K).NE.0.0) GOTO 99
      IF(IM(L)-IM(K).NE.0.0) GOTO 99
      IF(IL(L)-IL(K) .EQ.1.0) GOTO 11
      IF(IL(L)-IL(K) .NE.-1.0) GOTO 99
      IF(IV(L)-IV(K).EQ. 0.0) GOTO 22
      IF(IV(L)-IV(K).NE.1.0) GOTO 99
      ZILK      =(-1.0/ALPHA)*SQRT(IV(L))*S5(IL(L),IM(L))
      ZJKL      =(-1.0/ALPHA)*S2(IV(K))*S4(IL(K),IM(K))
      GO TO 100
   22 ZILK      =(1.0/ALPHA)*S3(IV(L),IL(L))*S5(IL(L),IM(L))
      ZJKL      =(1.0/ALPHA)*S1(IV(K),IL(K))*S4(IL(K),IM(K))
      GOTO 100
   11 IF(IV(L)-IV(K).EQ. -1.0) GOTO 33
      IF(IV(L)-IV(K).NE.0.0) GOTO 99
      ZILK      =(1.0/ALPHA)*S1(IV(L),IL(L))*S4(IL(L),IM(L))
      ZJKL      =(1.0/ALPHA)*S3(IV(K),IL(K))*S5(IL(K),IM(K))
      GO TO 100
   33 ZILK      =(-1.0/ALPHA)*S2(IV(L))*S4(IL(L),IM(L))
      ZJKL      =(-1.0/ALPHA)*SQRT(IV(K))*S5(IL(K),IM(K))
      GO TO 100
   99 ZILK=0.0
```

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         00000000011111111112222222222333333333344444444445555555555666666666677777777778
         12345678901234567890123456789012345678901234567890123456789012345678901234567890
               ZJKL=0.0
           100 ZIZJ=(-1.0)*ZILK*ZJKL
               IF(ZIZJ.EQ.0.0)GO TO 20
               SUMM=SUMM+ZIZJ
               WRITE(6,105)L,K,ZILK,ZJKL,ZIZJ ,SUMM
            20 CONTINUE
               ZIJWO=SUMM/(N*(N-1))
               WRITE(6,107)SUMM
               WRITE(6,106)ZIJWO
               STOP
               END
         $ENTRY
```

APPENDIX B

PROGRAM FOR THE REQUIRED MATRIX ELEMENTS IN THE CALCULATION OF σ_b WHEN EHO MODEL IS USED

This program will print out the same required matrix elements as the program given in Appendix A. The only difference is now the wave functions of EHO model are used in $|0\rangle$. The oscillator constant λ is included in this program.

$$\text{ZSQWO} = \langle 0|z_i^{\,2}|0\rangle$$

$$\text{ZIZJ} = \langle 0|z_i z_{i'}|0\rangle$$

The input data are the quantum numbers ν, κ and μ of each proton.

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00000000011111111112222222222333333333344444444445555555555666666666677777777778
12345678901234567890123456789012345678901234567890123456789012345678901234567890
$JOB
  101 FORMAT(3F5.1)
  102 FORMAT (1X,I5,4F10.1,5E15.4)
  103 FORMAT(1X,8HZSQWC IS,10X,E15.4)
  104 FORMAT(1X,2I5,5X,4E20.4)
  105 FORMAT(1X,9HZIZJWO IS,10X,E20.4)
      REAL V(130),K(130),U(130),L(130),E(130),CA(130),CB(130), O(130),
     1ZSQVKU(130),MC2,ZSQVNK(130)
      COA(A,B)=-1.0*SQRT(ABS((A-B+0.5)/(2.0*A+1.0)))
      COB(A,B)=SQRT(ABS((A+B+0.5)/(2.0*A+1.0)))
      COC(A,B)=SQRT(ABS((A+B+0.5)/(2.0*A+1.0)))
      COD(A,B)=SQRT(ABS((A-B+0.5)/(2.0*A+1.0)))
      COE(A,B)=SQRT(ABS((A+B-0.5)/(2.0*A-1.0)))
      COF(A,B)=SQRT(ABS((A-B-0.5)/(2.0*A-1.0)))
      COG(A,B)=-1.0*SQRT(ABS((A-B+1.5)/(2.0*A+3.0)))
      COH(A,B)=SQRT(ABS((A+B+1.5)/(2.0*A+3.0)))
      N=82
      A=208.0
      RM=1.67239*(10.0**(-24.0))
      C=2.9979*(10.0**10.0)
      H=1.05443*(10.0**(-27.0))
      VEM=1.6*(10.0**(-6.0))
      MC2=RM*C*C
      T=SQRT((42.0   *RM*VEM*(A**(-1.0/3.0)))/(H*H))
      THC=T*H*C
      SUM=0.0
      DO 10 I=1,N
      READ (5,101)V(I),K(I),U(I)
      O(I)=SQRT(MC2*MC2+4.0*THC*THC*(V(I)+ABS(K(I))+0.5))
      CA(I)=(1.0+((O(I)-MC2)**2)/(4.0*THC*THC*(V(I)+ABS(K(I))+0.5)))**(-
     10.5)
      CB(I)=((K(I)/ABS(K(I)))*(O(I)-MC2))/(2.0*THC*SQRT(V(I)+ABS(K(I))+0
     1.5))
      IF(K(I).GT.0.0) GO TO 11
      L(I)=-1.0*K(I)-1.0
      CALL SS(V(I),L(I),U(I)-0.5,S1)
      CALL SS(V(I),L(I),U(I)+0.5,S2)
      ZSQVKU(I)=((L(I)+U(I)+0.5)/(2.0*L(I)+1.0))*S1+(
     1(L(I)-U(I)+0.5)/(2.0*L(I)+1.0))*S2
      CALL SS(V(I),L(I)+1.0,U(I)-0.5,S3)
      CALL SS(V(I),L(I)+1.0,U(I)+0.5,S4)
      ZSQVNK (I)=((L(I)-U(I)+1.5)/(2.0*L(I)+3.0))*S3
     1   +((L(I)+U(I)+1.5)/(2.0*L(I)+3.0))*S4
      GO TO 22
   11 L(I)=K(I)
      CALL SS(V(I),L(I),U(I)-0.5,S5)
      CALL SS(V(I),L(I),U(I)+0.5,S6)
      ZSQVKU(I)=((L(I)-U(I)+0.5)/(2.0*L(I)+1.0))*S5
     1+((L(I)+U(I)+0.5)/(2.0*L(I)+1.0))*S6
      CALL SS(V(I),L(I)-1.0,U(I)-0.5,S7)
      CALL SS(V(I),L(I)-1.0,U(I)+0.5,S8)
      ZSQVNK(I)=((L(I)+U(I)-0.5)/(2.0*L(I)-1.0))*S7
     1  +((L(I)-U(I)-0.5)/(2.0*L(I)-1.0))*S8
   22 RZSQI=  CA(I)*CA(I)*ZSQVKU(I)+CA(I)*CA(I)*CB(I)*CB(I)*ZSQVNK (I)
```

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12345678901234567890123456789012345678901234567890123456789012345678901234567890
      SUM=SUM+RZSQI
      WRITE(6,102)I,V(I),K(I),U(I),L(I),CA(I),CB(I),D(I),RZSQI,SUM
   10 CONTINUE
      ZSQWC=SUM/N
      WRITE(6,103)ZSQWC
      SUMM=0.0
      DO 20 J=1,N
      DO 20 M=1,N
      IF(J.EQ.M) GO TO 20
      IF(K(J)) 202,202,121
  121 IF(K(M)) 44,44,33
   33 L(J)=K(J)
      L(M)=K(M)
      CALL AA(V(J),L(J),U(J)-0.5,V(M),L(M),U(M)-0.5,Z1)
      CALL AA(V(J),L(J),U(J)+0.5,V(M),L(M),U(M)+0.5,Z2)
      CALL AA(V(J),L(J)-1.0,U(J)-0.5,V(M),L(M)-1.0,U(M)-0.5,Z3)
      CALL AA(V(J),L(J)-1.0,U(J)+0.5,V(M),L(M)-1.0,U(M)+0.5,Z4)
      CALL AA(V(M),L(M),U(M)-0.5,V(J),L(J),U(J)-0.5,Z5)
      CALL AA(V(M),L(M),U(M)+0.5,V(J),L(J),U(J)+0.5,Z6)
      CALL AA(V(M),L(M)-1.0,U(M)-0.5,V(J),L(J)-1.0,U(J)-0.5,Z7)
      CALL AA(V(M),L(M)-1.0,U(M)+0.5,V(J),L(J)-1.0,U(J)+0.5,Z8)
      ZIVKLK      =COA(L(J),U(J))*COA(L(M),U(M))*Z1+COB(L(J),U(J))*COB(L(
     CM),U(M))*Z2
      ZIVNKL       =COE(L(J),U(J))*COE(L(M),U(M))*Z3+COF(L(J),U(J))*COF(L
     C(M),U(M))*Z4
      ZJVKKL      =COA(L(J),U(J))*COA(L(M),U(M))*Z5+COB(L(J),U(J))*COB(L(
     CM),U(M))*Z6
      ZJVNKK      =COE(L(J),U(J))*COE(L(M),U(M))*Z7+COF(L(J),U(J))*COF(L
     C(M),U(M))*Z8
      GO TO 100
   44 L(J)=K(J)
      L(M)=-1.0*K(M)-1.0
      CALL AA(V(J),L(J),U(J)-0.5,V(M),L(M),U(M)-0.5,Z11)
      CALL AA(V(J),L(J),U(J)+0.5,V(M),L(M),U(M)+0.5,Z12)
      CALL AA(V(J),L(J)-1.0,U(J)-0.5,V(M),L(M)+1.0,U(M)-0.5,Z13)
      CALL AA(V(J),L(J)-1.0,U(J)+0.5,V(M),L(M)+1.0,U(M)+0.5,Z14)
      CALL AA(V(M),L(M),U(M)-0.5,V(J),L(J),U(J)-0.5,Z15)
      CALL AA(V(M),L(M),U(M)+0.5,V(J),L(J),U(J)+0.5,Z16)
      CALL AA(V(M),L(M)+1.0,U(M)-0.5,V(J),L(J)-1.0,U(J)-0.5,Z17)
      CALL AA(V(M),L(M)+1.0,U(M)+0.5,V(J),L(J)-1.0,U(J)+0.5,Z18)
      ZIVKLK      =COA(L(J),U(J))*COC(L(M),U(M))*Z11+COB(L(J),U(J))*COD(L
     C(M),U(M))*Z12
      ZIVNKL       =COE(L(J),U(J))*COG(L(M),U(M))*Z13+COF(L(J),U(J))*COH(
     CL(M),U(M))*Z14
      ZJVKKL      =COA(L(J),U(J))*COC(L(M),U(M))*Z15+COB(L(J),U(J))*COD(L
     C(M),U(M))*Z16
      ZJVNKK      =COE(L(J),U(J))*COG(L(M),U(M))*Z17+COF(L(J),U(J))*COH(
     CL(M),U(M))*Z18
      GO TO 100
  202 IF(K(M)) 66,66,55
   55 L(J)=-1.0*K(J)-1.0
      L(M)=K(M)
      CALL AA(V(J),L(J),U(J)-0.5,V(M),L(M),U(M)-0.5,Z21)
      CALL AA(V(J),L(J),U(J)+0.5,V(M),L(M),U(M)+0.5,Z22)
```

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        00000000011111111112222222222333333333344444444445555555555666666666677777777778
        12345678901234567890123456789012345678901234567890123456789012345678901234567890
      CALL  AA(V(J),L(J)+1.0,U(J)-0.5,V(M),L(M)-1.0,U(M)-0.5,Z23)
      CALL  AA(V(J),L(J)+1.0,U(J)+0.5,V(M),L(M)-1.0,U(M)+0.5,Z24)
      CALL  AA(V(M),L(M),U(M)-0.5,V(J),L(J),U(J)-0.5,Z25)
      CALL  AA(V(M),L(M),U(M)+0.5,V(J),L(J),U(J)+0.5,Z26)
      CALL  AA(V(M),L(M)-1.0,U(M)-0.5,V(J),L(J)+1.0,U(J)-0.5,Z27)
      CALL  AA(V(M),L(M)-1.0,U(M)+0.5,V(J),L(J)+1.0,U(J)+0.5,Z28)
      ZIVKLK      =CCC(L(J),U(J))*CCA(L(M),U(M))*Z21+CCD(L(J),U(J))*CCB(L
     C(M),U(M))*Z22
      ZIVNKL      =COG(L(J),U(J))*CCE(L(M),U(M))*Z23+COH(L(J),U(J))*CCF(
     CL(M),U(M))*Z24
      ZJVKKL      =COC(L(J),U(J))*CCA(L(M),U(M))*Z25+CCD(L(J),U(J))*COB(L
     C(M),U(M))*Z26
      ZJVNKK      =COG(L(J),U(J))*CCE(L(M),U(M))*Z27+COH(L(J),U(J))*COF(
     CL(M),U(M))*Z28
      GO TO 100
   66 L(J)=-1.0*K(J)-1.0
      L(M)=-1.0*K(M)-1.0
      CALL  AA(V(J),L(J),U(J)-0.5,V(M),L(M),U(M)-0.5,Z31)
      CALL  AA(V(J),L(J),U(J)+0.5,V(M),L(M),U(M)+0.5,Z32)
      CALL  AA(V(J),L(J)+1.0,U(J)-0.5,V(M),L(M)+1.0,U(M)-0.5,Z33)
      CALL  AA(V(J),L(J)+1.0,U(J)+0.5,V(M),L(M)+1.0,U(M)+0.5,Z34)
      CALL  AA(V(M),L(M),U(M)-0.5,V(J),L(J),U(J)-0.5,Z35)
      CALL  AA(V(M),L(M),U(M)+0.5,V(J),L(J),U(J)+0.5,Z36)
      CALL  AA(V(M),L(M)+1.0,U(M)-0.5,V(J),L(J)+1.0,U(J)-0.5,Z37)
      CALL  AA(V(M),L(M)+1.0,U(M)+0.5,V(J),L(J)+1.0,U(J)+0.5,Z38)
      ZIVKLK      =COC(L(J),U(J))*COC(L(M),U(M))*Z31+COD(L(J),U(J))*COD(L
     C(M),U(M))*Z32
      ZIVNKL      =COG(L(J),U(J))*COG(L(M),U(M))*Z33+COH(L(J),U(J))*COH(
     CL(M),U(M))*Z34
      ZJVKKL      =COC(L(J),U(J))*COC(L(M),U(M))*Z35+COD(L(J),U(J))*COD(L
     C(M),U(M))*Z36
      ZJVNKK      =COG(L(J),U(J))*COG(L(M),U(M))*Z37+COH(L(J),U(J))*COH(
     CL(M),U(M))*Z38
      GOTO 100
  100 RZILK      =CA(J)*CA(M)*ZIVKLK      +CA(J)*CA(M)*CB(J)*CB(M)*
     CZIVNKL
      RZJKL      =CA(J)*CA(M)*ZJVKKL      +CA(J)*CA(M)*CB(J)*CB(M)*
     CZJVNKK
      IF(RZILK.EQ.0.0) GO TO 20
      IF(RZJKL.EQ.0.0) GO TO 20
      RZIZJ=(-1.0)*RZILK*RZJKL
      SUMM=SUMM+RZIZJ
      WRITE(6,104)J,M,RZILK,RZJKL,RZIZJ,SUMM
   20 CONTINUE
      B=N
      ZIZJ=SUMM/(B*(B-1.0))
      WRITE(6,105)ZIZJ
      STOP
      END
```

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0000000001111111111222222222233333333334444444444555555555566666666667777777778
1234567890123456789012345678901234567890123456789012345678901234567890123456789O
      SUBROUTINE AA(RVL,RLL,RML,RVK,RLK,RMK,ANS)
      S1(R1,R2)=SQRT(ABS(R1+R2+1.0/2.0))
      S2(R3)=SQRT(ABS(R3+1.0))
      S3(R4,R5)=SQRT(ABS(R4+R5+1.5))
      S4(R6,R7)=SQRT(ABS((R6*R6-R7*R7)/((2.0*R6+1.0)*(2.0*R6-1.0))))
      S5(R8,R9)=SQRT(ABS(((R8+1.0)*(R8+1.0)-R9*R9)/((2.0*R8+3.0)*
     C(2.0*R8+1.C))))
      ALPHA=1.0
      IF(ABS(RML).GT.RLL) GO TO 999
      IF(ABS(RMK).GT.RLK) GO TO 999
      IF(RML-RMK.NE.0.0) GO TO 999
      IF(RLL-RLK.EQ.1.C) GO TO 111
      IF(RLL-RLK.NE.-1.0) GO TO 999
      IF(RVL-RVK.EQ.0.0) GO TO 222
      IF(RVL-RVK.NE.1.0) GO TO 999
      ANS=(-1.0/ALPHA)*SQRT(ABS(RVL))*S5(RLL,RML)
      GO TO 777
  222 ANS=(1.0/ALPHA)*S3(RVL,RLL)*S5(RLL,RML)
      GO TO 777
  111 IF(RVL-RVK.EQ.-1.0) GO TO 333
      IF(RVL-RVK.NE.0.0) GO TO 999
      ANS=(1.0/ALPHA)*S1(RVL,RLL)*S4(RLL,RML)
      GO TO 777
  333 ANS=(-1.0/ALPHA)*S2(RVL)*S4(RLL,RML)
      GO TO 777
  999 ANS=0.0
  777 RETURN
      END

      SUBROUTINE SS(A,B,C,S)
      IF(ABS(C).GT.B) GO TO 1
      S=(-1.0)                    *(2.0*A+B+1.5)*(1.0/3.0)*(((2.0*(3.0*C*
     1C-B*(B+1.0)))/((2.0*B-1.0)*(2.0*B+3.0)))-1.0)
      GO TO 2
    1 S=0.0
    2 RETURN
      END
$ENTRY
```

APPENDIX C

PROGRAM FOR THE SUMMED OSCILLATOR STRENGTHS

The summed oscillator strengths, $\sum_{n'} f_{n'n}$, where $f_{n'n}$ was defined in Eq. (107) of Chapter VI were calculated using this program. For the given initial states,

$$SUM = \sum_{n'} f_{n'n} .$$

The input data cards include all the degenerate initial states of a given energy level and all the possible final states.

```
000000000111111111122222222223333333333444444444455555555556666666666777777777778
123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
CARD
$JOB
   101 FORMAT(3F5.1)
   102 FORMAT(1X,I5,3F10.1,5X,3E15.4)
   103 FORMAT(1X,2I5,2F20.4,10X,5HFOR X)
   104 FORMAT(1X,2I5,2F20.4,10X,5HFOR Y)
   105 FORMAT(1X,2I5,2F20.4,10X,5HFOR Z)
   106 FORMAT (1X,4F20.4)
       REAL V(130),K(130),U(130),L(130),O(130),CA(130),CB(130),MC2
       COA(A,B)=-1.0*SQRT(ABS((A-B+0.5)/(2.0*A+1.0)))
       COB(A,B)=SQRT(ABS((A+B+0.5)/(2.0*A+1.0)))
       COC(A,B)=SQRT(ABS((A+B+0.5)/(2.0*A+1.0)))
       COD(A,B)=SQRT(ABS((A-B+0.5)/(2.0*A+1.0)))
       COE(A,B)=SQRT(ABS((A+B-0.5)/(2.0*A-1.0)))
       COF(A,B)=SQRT(ABS((A-B-0.5)/(2.0*A-1.0)))
       COG(A,B)=-1.0*SQRT(ABS((A-B+1.5)/(2.0*A+3.0)))
       COH(A,B)=SQRT(ABS((A+B+1.5)/(2.0*A+3.0)))
       N=32
       A=63.0
       RM=1.67239*(10.0**(-24.0))
       C=2.9979*(10.0**10.0)
       H=1.05443*(10.0**(-27.0))
       VEM=1.6*(10.0**(-6.0))
       MC2=RM*C*C
       T=SQRT((42.0   *RM*VEM*(A**(-1.0/3.0)))/(H*H))
       THC=T*H*C
       DO 10 I=1,N
       READ (5,101)V(I),K(I),U(I)
       O(I)=SQRT(MC2*MC2+4.C*THC*THC*(V(I)+ABS(K(I))+0.5))
       CA(I)=(1.0+((O(I)-MC2)**2)/(4.0*THC*THC*(V(I)+ABS(K(I))+0.5)))**(-
      10.5)
       CB(I)=((K(I)/ABS(K(I)))*(O(I)-MC2))/(2.0*THC*SQRT(V(I)+ABS(K(I))+0
      1.5))
       WRITE(6,102) I,V(I),K(I),U(I),CA(I),CB(I),C(I)
    10 CONTINUE
       DO 60 J=1,12
       SUMX=0.0
       SUMY=0.0
       SUMZ=0.0
       SUM=0.0
       DO 20 M=1,N
       IF(O(J).EQ.O(M)) GO TO 20
       COEFF=(2.0*MC2)/(O(M)-O(J))
       IF (K(J).GE. 0.0 ) L(J)=K(J)
       IF (K(M).GE. 0.0 ) L(M)= K(M)
       IF (K(M).LE. 0.0) L(M)= (-1.0)*K(M)-1.0
       IF (K(J).LE. 0.0) L(J)= (-1.0)*K(J)-1.0
       AA=CA(J)
       AP=CA(M)
       BB=CB(J)
       BP=CB(M)
       A=COA(L(J),U(J))
       B=COB(L(J),U(J))
       C=COC(L(J),U(J))
       D=COD(L(J),U(J))
```

```
00000000011111111112222222222333333333344444444445555555555666666666677777777778
12345678901234567890123456789012345678901234567890123456789012345678901234567890
      E=COE(L(J),U(J))
      F=COF(L(J),U(J))
      G=COG(L(J),U(J))
      H=COH(L(J),U(J))
      AF=COA(L(M),U(M))
      BF=COB(L(M),U(M))
      CF=COC(L(M),U(M))
      DF=COD(L(M),U(M))
      EF=COE(L(M),U(M))
      FF=COF(L(M),U(M))
      GF=COG(L(M),U(M))
      HF=COH(L(M),U(M))
      IF (K(J)) 202,202,121
  121 IF (K(M)) 44,44,33
   33 L(J)=K(J)
      L(M)=K(M)
      IF ((U(M)+0.5).EQ.(U(J)-0.5)) GO TO 111
      IF ((U(M)-0.5).EQ.U(J)+0.5)  GO TO222
      IF (U(M).EQ.U(J)) GO TO 333
      GO TO 20
  111 IF (L(M).EQ.L(J)-1.0) GO TO 112
      IF (L(M)-1.0.EQ.L(J)) GO TO 113
      GO TO 20
  112 AAX=(AP*AA*BB*BF*E)
      AAY=(AP*AA*BB*BF*E)
      AAX=AAX*AAX
      AAY=AAY*AAY
      GO TO 99
  113 AAX=(AP*AA*BP*FF*A)
      AAY=(AP*AA*BP*FF*A)
      AAX=AAX*AAX
      AAY =AAY*AAY
      GO TO 99
  222 IF(L(M).EQ.L(J)-1.0) GO TO 223
      IF (L(M)-1.0 .EQ.L(J)) GO TO 224
      GO TO 20
  223 AAX=(AP*AA*BB*AF*F)
      AAX=AAX*AAX
      AAY=AAX
      GO TO 99
  224 AAX=(AP*AA*BP*EF*B)
      AAX=AAX*AAX
      AAY=AAX
      GO TO 99
  333 IF(L(M).EQ.L(J)-1.0) GO TO 334
      IF (L(M)-1.0.EQ.L(J)) GO TO 335
      GO TO 20
  334 AAZ1=AP*AA*BB*(E*AF-F*BF)
      AAZ=AAZ1*AAZ1
      GO TO 999
  335 AAZ1=AP*AA*BP*(EF*A-FF*B)
      AAZ=AAZ1*AAZ1
      GO TO 999
   44 L(J)=K(J)
```

```
0000000001111111111222222222233333333334444444444555555555566666666667777777777778
12345678901234567890123456789012345678901234567890123456789012345678901234567890
        L(M)=(-1.0)*K(M)-1.0
        IF(L(M).EQ.L(J)-1.0) GO TO 23
        GO TO 20
     23 IF (U(M)+0.5.EQ.U(J)-0.5) GO TO 21
        IF (U(M)-0.5.EQ.U(J)+0.5) GO TO 31
        IF (U(M).EQ.U(J)) GO TO 41
        GO TO 20
     21 AAX=AP*AA*(BB*E*CF-BP*HF*A)
        AAX=AAX*AAX
        AAY=AAX
        GO TO 99
     31 AAX=AP*AA*(BB*F*CF-BP*GF*B)
        AAX=AAX*AAX
        AAY=AAX
        GO TO 99
     41 AAZ=AP*AA*(BB*(E*CF-F*DF)-BP*(A*GF+B*HF))
        AAZ=AAZ*AAZ
        GO TO 999
    202 L(J)=(-1.0)*K(J)-1.0
        IF (K(M)) 55,55,66
     66 L(M)=K(M)
        IF (L(M).EQ.L(J)+1.0) GO TO 67
        GO TO 20
     67 IF (U(M)+0.5 .EQ. U(J)-0.5) GO TO 71
        IF (U(M)-0.5 .EQ. U(J)+0.5) GO TO 72
        IF (U(M).EQ. U(J)) GO TO 73
        GO TO 20
     71 AAX=AP*AA*(BB*G*BF-BP*FF*C)
        AAX=AAX*AAX
        AAY=AAX
        GO TO 20
     72 AAX=AP*AA*(BB*H*AF-BP*D*EF)
        AAX=AAX*AAX
        AAY=AAX
        GO TO 99
     73 AAZ=AP*AA*(BB*(G*AF-H*BF)-BP*(C*EF-D*FF))
        AAZ=AAZ*AAZ
        GO TO 999
     55 L(M)=(-1.0)*K(M)-1.0
        IF (U(M)+0.5.EQ.U(J)-0.5) GO TO 51
        IF (U(M)-0.5.EQ.U(J)+0.5) GO TO 52
        IF (U(M).EQ.U(J)) GO TO 53
        GO TO 20
     51 IF (L(M).EQ.L(J)+1.0) GO TO 54
        IF (L(M).EQ.L(J)-1.0) GO TO 56
        GO TO 20
     54 AAX=(AP*AA*BB*G*CF)
        AAX=AAX*AAX
        AAY=AAX
        GO TO 99
     56 AAX=(AP*AA*BP*C*HF)
        AAX=AAX*AAX
        AAY=AAX
        GO TO 99
```

```
000000000111111111122222222223333333333444444444455555555556666666666777777777778
12345678901234567890123456789012345678901234567890123456789012345678901234567890
      52 IF (L(M).EQ.L(J)+1.0) GO TO 58
         IF (L(M)+1.0.EQ.L(J)) GO TO 59
         GO TO 20
      58 AAX=(AP*AA*BB*H*CF)
         AAX=AAX*AAX
         AAY=AAX
         GO TO 99
      59 AAX=(AP*AA*BP*D*GF)
         AAX=AAX*AAX
         AAY=AAX
         GO TO 99
      53 IF (L(M).EQ.L(J)+1.0) GO TO 531
         IF (L(M)+1.0.EQ.L(J)) GO TO 532
         GO TO 20
     531 AAZ=AA*AP*BB*(G*CF-H*DF)
         AAZ=AAZ*AAZ
         GO TO 999
     532 AAZ=AA*AP*BP*(C*GF-D*HF)
         AAZ=AAZ*AAZ
         GO TO 999
      99 AAX=COEFF*AAX
         SUMX=SUMX+AAX
         WRITE(6,103)J,M,AAX,SUMX
         AAY=AAY*COEFF
         SUMY=SUMY+AAY
         WRITE(6,104)J,M,AAY,SUMY
         GO TO 20
     999 AAZ=AAZ*COEFF
         SUMZ=SUMZ+AAZ
         WRITE(6,105)J,M,AAZ,SUMZ
      20 CONTINUE
         SUM=SUMX+SUMY+SUMZ
         WRITE(6,106) SUMX,SUMY,SUMZ,SUM
      60 CONTINUE
         STOP
         END
$ENTRY
```

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