CHAPTER II

BRIEF THEORY OF ISOTOPE SHIFT
2.1 Introduction

The energy levels of two different isotopes of a given element have slightly different values, this difference observable in an atomic spectral line (usually under high resolution) is termed "isotope shift".

Isotope shift between two isotopes $A$ and $A'$ in a spectral line of frequency $\nu$ is given by

$$\Delta \nu_{IS} = \nu^A - \nu^{A'}$$  \hspace{1cm} (1)

The energy of the transition is different for two isotopes which differ only in nuclear mass but having the same nuclear and electronic charge. If two isotopes are labelled $H$ for heavy and $L$ for light

$$E'_H - E''_H = h\nu_H \text{ and } E'_L - E''_L = h\nu_L$$

and the difference

$$h\nu_H - h\nu_L = h\Delta \nu$$

is the isotope shift (IS)

$$IS = (E'_H - E''_H) - (E'_L - E''_L)$$  \hspace{1cm} (2)

Isotope shift in atomic spectral line can be either as
a consequence of differences in the nuclear masses of the isotopes \( A \) and \( A' \), or on account of the difference in the nuclear charge distribution of the two isotopes \( A \) and \( A' \). The former is known as the 'mass effect' and the latter as the 'field effect' \([1]\), which are described in the following sections.

2.2 Mass Effect

Each atomic level is described by an eigenfunction with eigen value of angular momentum and energy. The angular momentum of an energy level has a definite fixed value for all isotopes, so if the mass of the atomic nucleus is changed, the energy of the level will have to change so that the angular momentum can remain the same. This change in the energy eigen value of a level due to change in the mass of the nucleus is generally known as the mass shift (also referred as Bohr shift or the reduced mass effect).

The Hamiltonian \( H_0 \) of an one-electron atom with infinite nuclear mass, that is, considering the nucleus to be stationary, is given \([2]\) as

\[
H_0 = \frac{-\hbar^2}{2m_e} \nabla^2 + V(r)
\]  

(3)
where \( m_e \) is the mass of the electron, \( V(r) \) includes the Coulomb interaction between the electron and the nucleus (neglecting the spin dependence and relativistic effect). Solving the Schrödinger equation

\[
H \psi = E \psi \tag{4}
\]

with \( H \) in (3), the energy eigenvalues for the simplest atom can be given as

\[
E = - R_\infty \frac{Z^2}{n^2} \tag{5}
\]

where \( Z \) is the nuclear charge and \( n \) is the principle quantum number, the Rydberg constant \( R_\infty = \frac{m_e e^4}{2\hbar^2} \) includes only the mass of the electron, the suffix \( \infty \) indicating the finiteness of the nuclear mass which has to be considered for evaluating the energy eigenvalues. By taking into account the motion of the nucleus about the common centre of the gravity of the nucleus and the electron, we have

\[
H_0 = -\frac{\hbar^2}{2m_e} \nabla^2 + \frac{P}{2\hbar} + V(r) \tag{6}
\]
where \( P \) is the momentum of the nucleus, \( M \) is mass of the nucleus. Now reduced mass \( \mu \) is defined as
\[
\mu = \frac{m \cdot M}{m + M}
\]
equation (6) can be written as
\[
H = -\frac{\hbar}{2\mu} \nabla^2 + V(r)
\]  
(7)

Solving the Schrödinger equation with the Hamiltonian as in eq (7), the energy eigen values are
\[
E_n = -R_\infty \left( \frac{M_n}{m + M_n} \right) \frac{Z^2}{n^2}
\]  
(8)

This difference in energy due to reduced mass correction is known as normal mass shift (NMS). The NMS in a transition \( \nu \) between isotopes of mass \( A \) and \( A' \) is
\[
\Delta \nu_{\text{NMS}} = \nu \frac{A - A'}{AA'} \times 5.49 \times 10^{-4} \text{ cm}^{-1}
\]  
(9)

where \( \nu \) is in cm\(^{-1}\). For example, in the Balmer \( \alpha \) line the shift between \(^2\text{H} \) and \(^1\text{H} \) is 22.4 cm\(^{-1}\), or 671 GHz, or 1.79 \( \AA \) [3].
2.3 Specific Mass Shift

In many electron-spectra the electron momenta may be correlated. This correlation is determined not just by the energy of the level concerned but also by the specific properties of that level. So this extra mass shift is called the 'specific mass shift' (SMS). It is usually small, compared with the normal mass shift of a level, and can be treated as a perturbation. The total kinetic energy of N electrons and nucleus of mass M is [4]

\[ E_k = \sum_i \frac{p_i^2}{2m_e} + \frac{P^2}{2M} \]  \hspace{1cm} (10)

where \( p_i \) and \( P \) are the momentum of the electron and nucleus respectively. Relative to the centre of mass of the atoms, \( P = -p_i \), as the total momenta is zero.

\[ E_k = \sum_i \frac{p_i^2}{2m_e} + \frac{\Sigma (p_i)^2}{2M} \]  \hspace{1cm} (11)

\[ = \sum_i \frac{p_i^2}{2m_e} + \frac{1}{M} \left[ \Sigma_j p_i p_j \right] \]  \hspace{1cm} (12)

\[ = \sum_i \frac{p_i^2}{2\mu} + \frac{1}{M} \left[ \Sigma_j p_i p_j \right] \]  \hspace{1cm} (13)

The Hamiltonian for the multi-electron atom can be rewritten as
Thus in a multi-electron atom, there is an additional ‘coupling effect’ of the momentum correlation terms in (7), which produces different shifts for different energy levels. The first order perturbation energy is given by

$$\Delta W = \frac{\hbar^2}{M} \sum_{i,j} \int \psi_i^* \nabla_i \psi_j \, dr$$

(15)

The correction due to specific mass shift is given as [4]

$$\delta \omega_{\text{SMS}}^{AA'} = S \frac{A - A'}{AA'}$$

(16)

in equation (6). The correction to the energy eigen values due to the mass effect as a whole, is obtained and given by

$$\delta \omega_{\text{SM}}^{AA'} = N \frac{A - A'}{AA'} + S \frac{A - A'}{AA'}$$

(17)

N being the parameter due to the normal mass effect and S due to specific mass effect.

The NMS is always positive, as N is always greater than zero. The specific mass shift originates from the influence of correlations in the motion of the recoil energy of the
nucleus, thus the factor $S$ can be either positive or negative depending on the correlations between all the electrons in the atom.

Both NMS and SMS are inversely proportional to the square of the mass number $A$, i.e., $1/A^2$, yet appreciable SMS is observed in the heavy elements. For light elements ($Z \leq 30$) the observed IS can be practically considered to be the sum of NMS and SMS [5]. Therefore, for these elements the specific mass shift can be easily deduced from the observed isotope shift.

2.4 Field Shift due to Extended Nuclear Charge Distribution

The nuclear volume effect becomes significant in heavy elements starting from around molybdenum ($A = 98$) and going right up to the end of the periodic table.

So far in our discussion, the nucleus has been treated as a point charge; whereas the nucleus actually occupies a finite volume over which the positive charge is distributed and it is possible for the electron to move inside this charge. The interaction of the electrons with the modified nuclear potential results in what is known as the field shift.
(FS). Field shift arises due to the change of the finite size and angular shape of the nuclear charge distribution when the neutrons are added to the nucleus, consequently the binding energy of the electrons which penetrates the nucleus differ for different isotopes.

When the nucleus is considered to have an extended charge distribution, with charge density $\rho_n(r)$ and if $\rho_e(r)$ is the external charge density due to the changes in the atomic system, the electrostatic interaction energy is given by [6]

$$ W = \iint \frac{\rho_n(r)\rho_e(r')}{|r - r'|} \, dr \, dr' \tag{18} $$

The field shift $\Delta \nu_{FS}$ between the two isotopes $A$ and $A'$ during an electronic transition between two levels $e_1$ and $e_2$ is given by

$$ \Delta \nu_{FS} = -e^2 \iint \frac{1}{|r - r'|} \times \left[ \rho_A(r) \rho_{e1}(r') - \rho_A(r) \rho_{e2}(r') + \rho_{A'}(r) \rho_{e2}(r') + \rho_{A'}(r) \rho_{e1}(r') \right] \tag{19} $$

where $\rho_A$ and $\rho_{A'}$ is the nuclear charge distribution of the two isotopes $A$ and $A'$. Usually a spherical nucleus is assumed which changes the denominator from $|r - r'|$ to $r$, which means the larger of the two values $|r|$ and $|r'|$ during the
integration. The electron density within the nucleus is expressed as a

\[ \rho_e = a_0 + a_2 r^2 + a_4 r^4 + \ldots \quad (20) \]

Expanding the denominator in terms of spherical harmonics with \( |r| > |r'| \) we have

\[ |r-r'| = 4\pi \sum_{l=0}^{\infty} \sum_{m=1}^{l} \frac{1}{2l+1} \frac{1}{r^l} \left( \frac{r}{r'} \right)^l Y_{lm}^*(r)Y_{lm}(r') \quad (21) \]

For illustration, consider only the first integral

\[ = -e^2 \int \int dr \, dr' \frac{\rho_\Lambda(r) \rho_{e1}(r')}{|r-r'|} \quad (22) \]

of equation (19) and substituting equations (20) and (21) in this we get

\[ \frac{2\pi}{3} ze^2 a_0 \langle r^2 \rangle^\Lambda + \frac{\pi}{5} ze^2 a_2 \langle r^4 \rangle^\Lambda + \frac{2\pi}{21} ze^2 a_4 \langle r^6 \rangle^\Lambda + \ldots \quad (23) \]

If the difference of the four integrals in eq. (19) is taken we have the expression for the field shift

\[ \delta \nu_{FS}^{\Lambda\Lambda'} = \frac{2\pi}{3} ze^2 \left[ \Delta a_0 \delta \langle r^2 \rangle^\Lambda^\Lambda' + \frac{3}{10} \Delta a_2 \delta \langle r^4 \rangle^\Lambda^\Lambda' + \right. \\
\left. + \frac{1}{7} \Delta a_4 \delta \langle r^6 \rangle^\Lambda^\Lambda' + \ldots \right] \quad (24) \]
with $\Delta a_o$ as the difference of the electronic densities in the two configurations at $r = 0$, usually written as $\Delta |\psi(0)|^2$ and $\delta\langle r^n \rangle^{AA'}$ the difference of the expectation values of $r^n$ over the nuclear charge distribution of the two nuclei i.e,

$$\delta\langle r^n \rangle^{AA'} = \int \rho_A \langle r \rangle r^n \, dr - \int \rho_A' \langle r \rangle r^n \, dr$$  \hspace{1cm} (25)

Eq (23) can be re-written as

$$\delta\mu_{FS}^{AA'} = \frac{2\pi}{3} Z e^2 \Delta a_o \left[ \delta \langle r^2 \rangle^{AA'} + \frac{3}{10} \frac{\Delta a}{\Delta a_o} \delta \langle r^4 \rangle^{AA'} + \frac{1}{7} \frac{\Delta a}{\Delta a_o} \delta \langle r^4 \rangle^{AA'} + \ldots \right]$$  \hspace{1cm} (26)

$$= \frac{2\pi}{3} Z e^2 \Delta |\psi(0)|^2 (\lambda^{AA'})$$  \hspace{1cm} (27)

$$= F_i \lambda^{AA'}$$  \hspace{1cm} (28)

where $\lambda^{AA'} = \delta\langle r^2 \rangle^{AA'} + \frac{C_2}{C_1} \delta\langle r^4 \rangle^{AA'} + \frac{C_3}{C_4} \delta\langle r^6 \rangle^{AA'} + \ldots$  \hspace{1cm} (29)

where $\Delta a_z/\Delta a_o$ and $\Delta a_4/\Delta a_o$ values are expressed as the coefficients $C_z/C_1$ and $C_4/C_1$ respectively. As the S-wave function of the electron at the nucleus is largely independent of the principal quantum number, the relative contributions of the different moments to the FS are nearly equal for $K$ x-ray and optical transitions, therefore these ratios $C_n/C_1$ can be obtained from the $C_n$ values given for the $K$ x-ray shift by Seltzer [7].
The field shift depends on the electronic factor $F_e$ and the nuclear factor $\lambda^{AA'}$ and thus it can be used to obtain information concerning electronic configuration of the energy levels involved in the transition and also determine the changes in the nuclear charge distribution between isotopes. FS is mostly predominant in heavier elements ($A \geq 100$). FS can be observed only in transitions with $\Delta|\psi(0)|^2 \neq 0$. These comprise not only the transitions with an $s$-electron jump (or to a small extent with a $p_{1/2}$ -electron jump) but also transitions in which the screening of the inner closed $s$-electron is changed.

2.5 Screening parameters of Charge Density of s-electrons

The size of the field shift in a transition is proportional to the change in the total electron density at the nucleus. To a first approximation, this change is the change in the density at the nucleus of transition electron. In addition the density of the other electrons may change because of the change in the transition electron. Thus in heavy elements appreciable isotope shifts in a spectral line are to be expected only if the number of $s$ or $p_{1/2}$ electrons differs in two configurations involved in the transition. For example the FS in $d^2p - d^2s$ transition is much less than that
in dp-ds, because the additional 'd' electron screens the 's' electron much more from the nucleus, thereby reducing the charge density of the 's' electron at the nucleus. The FS in $s^2$-$d^2$ transition is not as large as in the transition of the type s-d as in the former the two 's' electrons screen each other thereby reducing the total effective electron charge density at the nucleus. Blaise and Steudal [8] have extended this analogy to the 5f series. They have also pointed out that, because of the screening of the closed 's' electron, the FS in a transition nf$^{m-1}$ to $(n+1)dnf^m$ is of the same order of magnitude as the field shift of an alkali like 's' electron in nf$(n+2)s$ ($n = 4,5$). This screening effect can be incorporated in the FS expression as the screening factor $\beta$ [1].

\[
\text{i.e. } \frac{\delta \nu^{AA'}}{\text{FS}} = \frac{\pi \alpha^3}{z} \beta \Delta |\psi(o)|^2 \times (\lambda^{AA'})
\]  

(30)

\[
\Delta |\psi(o)|^2 \text{ (all electrons considered)} = \beta \Delta |\psi(o)|^2 \text{ (of s-electrons)}
\]

If we omit the small contribution of an np$^{1/2}$ electron for which the charge density can be calculated as a fractional part of $|\psi(o)|^2_{ns}$ we can write for the total change of $|\psi(o)|^2$ in a (core + ns) - (core + np) transition as [9]
\[ \Delta |\psi(o)|_{ns-np}^2 = |\psi(o)|_{\text{core}}^2 + |\psi(o)|_{ns}^2 - |\psi(o)|_{\text{core}}^2 - |\psi(o)|_{np}^2 \]

\[ \sim \beta |\psi(o)|_{ns}^2 \quad \text{(31)} \]

with \[ \beta \sim \frac{|\psi(o)|_{\text{core}}^2 + |\psi(o)|_{ns}^2 - |\psi(o)|_{\text{core}}^2}{|\psi(o)|_{ns}^2} \]

The screening factor \( \beta \) takes into account the change in the screening of the inner closed-shell electrons from the nuclear charge by the valence electron as it changes from \( ns \) to \( np \). These screening factors theoretically are taken from non-relativistic Hartree-Fock [10]. On the basis of experimental observations, certain empirical relations have been established for the screening effect of \( s, p, d \) and \( f \) electron on the charge density of the ‘s’ electron at the nucleus. The extent to which other valance electrons screen the \( ns \) electron compared to a lone \( ns \) electron is obtained by the experimentally observed ratios of several pairs of configurations.

\[ \frac{\Delta T(ns^2)}{\Delta T(ns)} = 1.6 \quad \text{(32)} \]

\[ \frac{\Delta T(ns \, np)}{\Delta T(ns)} = 0.9 \quad \text{(33)} \]

\[ \frac{\Delta T(ns \, (n-1)d)}{\Delta T(ns)} = 0.8 \quad \text{(34)} \]
\[ \frac{\Delta T(ns (n+1)s)}{\Delta T(ns)} = 1.05 \quad (35) \]

The theoretical calculations of the screening factor \( \beta \) obtained by Hartree-Fock method agree well with the experimental deductions [10, 11]. Based on these screening ratios, the isotope shift value of any configuration can be approximately predicted if \( \Delta T \) of a particular configuration is known. Furthermore, the screening factors are of great value in understanding the observed isotope shifts in complex spectra with configuration mixing.

2.6 Isotope Shift and Electronic Configuration Mixing

In the absence of an external field, configurations can interact if they have the same parity. Within two such configurations, only levels of the same \( J \) can interact with one another. In complex spectra e.g., that of rare-earths, there are several valence electrons and many excited states have comparable energies, thus probability of configuration mixing is very large.

Energy level, therefore, can not be uniquely described by a single well defined wavefunction, due to configuration
mixing. In such cases, the isotope shift in a particular transition is a sensitive parameter to verify the configuration mixing. The IS of a level with mixed configuration has been derived by the application of the "sharing rule". According to this rule, for a state whose wavefunction $\Psi$ results from mixing of $n$ configurations, the isotope shift $\Delta T_i$ of the individual configurations is multiplied by the weight $C_i^2$ of the configurations in $\Psi$:

$$\Delta T = \sum_{i=1}^{n} C_i^2 \Delta T_i$$

(36)

where $\sum C_i^2 = 1$

The approximate validity of this rule was guessed by Jones [12], and Brix and Linderberger [13] (see our discussions on configuration mixing in Dy II energy levels under chapter 9).

2.7 Crossed - Second - Order Effect in Field Shift

To the first, order the mass shift (MS) as well as the field shift (FS) is a constant within a pure Russel - Saunders (RS) term of a particular configuration. This is the basis for grouping the energy levels according to their term shift $\Delta T$, which enables one to check or assign the electronic configurations to the energy levels. The $\Delta T$ values for
different terms of a pure configuration, are evaluated relative to a reference level and then separated into MS and FS. There may be slight difference in MS or FS for different RS terms of a particular configuration. This difference has been attributed to the influence of second-order contributions [14] to the isotope shift of a particular level.

Crossed-second-order effects in the field shifts mainly manifests in the $nl^N_{ns}$ type of configuration where the coupling of the 's' electron to the $l^N$ core causes the splitting of the RS terms into $M+l_1$ and $M-l_1$ terms (M being the multiplicity of total angular momentum L of the parent term resulting from the $l^N$ electrons) [14]. CSO effect leads to different electron charge densities for these two terms resulting in different FS values for these terms.

CSO contributions of the FS operator $F$ and the Electostatic operator $G$ to the total IS of a monoconfiguration state described by the wave function $\psi_0$ can be written as [5]

$$E_{\text{CSO}} = \sum_x \frac{\langle \psi_x | G | \psi_x \rangle \langle \psi_x | F | \psi_0 \rangle + \langle \psi_0 | F | \psi_x \rangle \langle \psi_x | G | \psi_x \rangle}{E_0 - E_x}$$

(37)
where $E_0$ and $E_x$ are the zeroth-order energies of the configurations $C_0$ and $C_x$ containing the states $\psi_0$ and $\psi_x$ respectively. The summation extends over all the states $\psi_x$ of all the configurations $C_x$ with sufficiently large energy difference $E_0 - E_x$ in order to enable a rapid convergence of the perturbation expression.

2.8 Relativistic Effects in $J$-dependence of Isotope Shift

The isotope shifts in heavy elements, due to nuclear volume effect, is mainly for levels involving s-electrons which have appreciable charge density at the nucleus. Due to relativistic effect (in high Z elements) there is contribution from $p_{1/2}$ electron; therefore it is expected that isotope shifts in transitions $D_1$ ($ns^2S_{1/2} - np^2P_{1/2}$) and $D_2$ ($ns^2S_{1/2} - np^2P_{3/2}$) will be different. The difference can be attributed to a relativistic effect on the $p_{1/2}$ wave functions, whose small Dirac component has the character of radial s-wavefunction, and this exhibit a nuclear volume effect. Fradkin [15] and Ionescu-Pallas [16] used hydrogenic wave functions to estimate this effect and obtained

$$
\sigma_H = (\alpha^2Z^2) / \{1 + (1 - \alpha^2Z^2)^{1/2}\}^2
$$

(38)
where $\alpha$ is (the ratio of FS in the two transitions of interest) expressed in percentage. Wendt et al [17] has used this wave function to estimate the J-dependance of the IS in the 6s - 6p doublet of Ba II. Experimentally they observed that the FS of the transition $6s^2S_{1/2} - 6p^2P_{3/2}$ is $2.5(3)\%$ smaller than that of transition $6s^2S_{1/2} - 6p^2P_{1/2}$. Theoretically estimating this effect using hydrogenic wave function they found that there is an over estimate of the effect by almost a factor of 2. This discrepancy is due to the omission of the effects of the screening of the core electrons on the $^2S_{1/2}$ and $^2P_{1/2}$ wave functions. Thus transitions involving $^2P_{1/2}$ and $^2P_{3/2}$ electrons from a common upper level would show a slight difference in the FS due to this relativistic effect.

By using the relativistic Dirac-Fock formalism the FS J-dependance in the transition of Yb$^+$ has been reported by Torbhom et al [6]. IS studies in Yb$^+$ has been carried out to verify these theoretical calculations relativistic effects (see chapter 5).
2.9 Isotope Shifts and Evaluation of Nuclear Parameter

2.9.1. Isotope Shift and Changes in Nuclear Charge Radii

Isotope Shift studies is the source of information regarding sizes and shape of nuclear charge distribution [18,19]. The variation of nuclear mean square charge radii, \( \delta \langle r^2 \rangle \) within the sequence of isotope, mainly reflects the changes in the collective property of these nuclei as a function of neutron numbers [(18,20 and references therein)]. It was the observation of sudden jump in isotope shifts in spectral lines of rare-earths which led to the concept of static deformation for nuclei having \( I=0^+ \) and provided the basis for the development of the collective model of the nuclei. On the basis of scattering studies [21], there are several expressions for charge distributions. To study the nuclear charge distribution, we concentrate on the moments of distribution rather than a single functional form.

The different moments of distribution are given by

\[
\langle r^n \rangle = \int \rho(r) \ r^n \ \text{d}^3r
\]  

(39)

The second moment of charge distribution is important for IS
studies [22] and it is given by

\[ \langle r^2 \rangle = \int \rho(r) r^2 \, d^3r \quad (40) \]

The direct determination of the total \( \langle r^2 \rangle \) of a nucleus from a given electronic term is very difficult, as the finite nuclear size affects the electronic spectra. Thus for the various isotopes, the interaction of nuclear charge distribution with the electronic charge density at the nucleus is different. The difference in interaction energy for two isotopes \( A \) and \( A' \) gives the field shift in a transition

\[ \delta u_{FS}^{AA'} = (\pi a_0^3/Z) \Delta \psi(\phi) f(Z) \delta \langle r^2 \rangle^{AA'} \quad (41) \]

\( FS \) can be factorised into two parts, nuclear and electronic part. By keeping electronic factor constant (measuring IS in a particular transition in a long chain of isotopes), we get information on the variation of the mean square charge radii \( \delta \langle r^2 \rangle^{AA'} \).

2.9.2 Relativistic Corrections and Evaluation of \( f \) Factor

The relativistic correction is obtained by
factorisation of change of electron charge density at the nucleus $\Delta |\psi(0)|^2$ into the product of the difference of the total non-relativistic charge density for a point nucleus and $f(Z)$, where function $f(Z)$ accounts for the relativistic correction to $E_i$ for a particular type of nuclear charge distribution i.e.

$$F_i = -\frac{2\pi}{3} Ze^2 \Delta |\psi(0)|^2 = \langle na_o^9/Z \Delta |\psi(0)|^2 f(Z) \rangle \quad (42)$$

$$= E_i f(Z) \quad (43)$$

where $E_i$ is the electronic factor in transition $i$, $f(Z)$ increases with $Z$.

For a finite nucleus size, the function $f(Z)$ contains the details of Dirac small large radial function. $f(Z)$ is derived from the isotope shift constant $C_{\text{unif}}$, which is given as

$$C_{\text{unif}} = \frac{\delta \nu_{\text{unif}}}{E_i} \quad (44)$$

Blundell et al. [23] have given the expression for $C_{\text{unif}}$ for the isotope pair.
\[ C_{\text{unif}}^{AA'} = (A' - A) C_{\text{unif}}^{A+1,A} + \beta(Z). \]

\[
\left[ \left( A^{2Y/3} - A'^{2Y/3} \right) - (A' - A) \left( (A+1)^{2Y/3} - A^{2Y/3} \right) \right]
\]

(45)

where \( \gamma = (1-z^2)^{1/2} \), \( \alpha \) is fine structure constant.

Zimmermann [24] has given improved expressions which include the contribution to the higher order radial moments of the nuclear charge distribution at least within 1% of \( C_{\text{unif}} \). Hence the expression for \( f(Z) \) is given as

\[
F(Z) = C_{\text{unif}} / \lambda_{\text{unif}}
\]

(46)

\[
\lambda_{AA'}^{AA'} = \sum_n C_n / C_{1} - \delta \left< r^{2n} \right>_{AA'}
\]

(47)

\[
F(Z) = C_{\text{unif}} / \sum_n C_n / C_{1} \cdot 2n/n+3 \cdot R_o^{2n} \tilde{A}^{(2n/3)-1} (A' - A)
\]

(48)

where \( \tilde{A} = (A+A)/2 \). These relations form the basis of semi-emperical evaluation of \( \lambda_{AA'}^{AA'} \). Babushkin [25] and Zimmermann [26] have given an expression for \( f(Z) \) but their expressions are differ from eq.(48), as the former calculatoins are made with the assumption that \( \lambda_{AA'}^{AA'} \approx \delta <r^2> \).
As the s-wavefunction at the nucleus is largely independent of the principal quantum number, the relative contribution of different moments to the field shift are nearly equal for K x-ray and optical transition. Therefore, the ratios $C_n/C_4$ can be obtained from $C_n$ values given for K x-ray shifts by Seltzer [7].

After evaluating F factor, the nuclear parameter can be obtained.

2.9.3 Changes in the Mean Square Charge Radii and Nuclear Deformation

The field effect of isotope shift measures the change of mean square charge distribution. So it is mainly governed by nuclear properties. According to nuclear model with saturated short range binding, nuclear volume is proportional to the mass number and hence $\langle r^2 \rangle$ is proportionate to $A^{2/3}$. In case of rare-earths $\delta \langle r^2 \rangle$ is not a smooth function of $A$ [18] (described in section 2.9.1). Thus the change in $\langle r^2 \rangle$ between isotopes, $\delta \langle r^2 \rangle$ can arise from changes in nuclear shape as well as in nuclear volume. This shape dependence has a strong and sometimes even abrupt $A$-dependence as a consequence of sudden transition from spherical to strongly
deformed nuclear shape.

The surface of an axially symmetric deformed and uniformly charge nucleus can be obtained from a spherical one by the following transformation [27].

\[ R_d = R_0 \, n \left( 1 + \sum_i \beta_i Y_i(\theta) \right) \]  

(49)

where parameters \( \beta_i \) are measure of multipole deformations of order \( i \), \( n \) is the normalization factor of \( \beta_i \). The mean square radius of a spheroid which has the same volume as a sphere with \( \langle r^2 \rangle \) is given as

\[ \langle r^2 \rangle = \langle r^2 \rangle_0 \left[ 1 + \frac{5}{4\pi} \right] \sum \langle \beta_i^2 \rangle \]  

(50)

\( \langle \beta_i \rangle \) represents an average deformation parameter arising from either zero-point vibration or static deformation with \( \langle \beta_i^2 \rangle = \beta_i \). The contribution due to quadrupole deformation parameter \( \beta_2 \), which is usually the predominant nuclear deformation, is expressed as

\[ \delta \langle r^2 \rangle = \delta \langle r^2 \rangle_0 + \frac{5}{4\pi} \langle r^2 \rangle_0 \delta \langle \beta_2^2 \rangle \]  

(51)

The evaluation of \( \beta_2 \) from observed \( \delta \langle r^2 \rangle \) has been discussed [28], where as the influence on \( \delta \langle r^2 \rangle \) of higher order
deformations like octupole $\beta_3$, hexadecapole ($\beta_4$) has been treated by Ahmad et al [29].
References

[1]. K. Heilig and A. Steudel, Atomic Data and Nuclear Data Tables, vol 14, No 5, 6 1974


