Chapter 2

Lifetime Determination and Theoretical Descriptions

2.1. Lifetime Determination

The time of flight method, variation of intensities of a certain transition with distance of the foil from entrance slit of the spectrometer, is used to take an intensity decay curve for lifetime measurements. Total flight length ranges from 2 to 10 decay lengths (ντ) starting at zero position of the foil. The experimentally observed decay curve is analyzed in the following way.

The decay rate from a state |i> having population \( N_i(t) \) at certain time, \( t \), is

\[
\frac{dN_i(t)}{dt} = -\lambda N_i(t) = -\frac{N_i(t)}{\tau_i} = -\sum_{j=1}^{n} A_{ij} N_j(t)
\]

(2.1)

where \( \lambda \) is the decay constant, \( \tau_i \) is the mean lifetime of the state |i> and \( A_{ij} \) is the transition probability for the spontaneous decay from state |i> to state |j>.

Integrating equation (2.1) from time \( t=0 \) to a given time \( t \), one gets

\[
N_i(t) = N_i(0) e^{-\frac{t}{\tau_i}}
\]

(2.2)

Where \( N_i(0) \) is the population of the state |i> at \( t=0 \) i.e., at the zero foil position. Let us now consider the simplest case of cascade or feeding which generally arises in the beam-foil interaction. Assume that a single upper level |k> cascades into the state |i> with the transition probability \( A_{ki} \) and \( A_{ki} =1/\tau_k \) with unity
branching ratio. Under these conditions the rate equation of the population of state $|i\rangle$ is

$$\frac{dN_i(t)}{dt} = -\frac{N_i(t)}{\tau_i} + \frac{N_k(t)}{\tau_k} \tag{2.3}$$

The solution of this differential equation is

$$n_i(t) = \left[ n_i(0) - n_k(0) \frac{\tau_i}{\tau_k - \tau_i} \right] e^{-\frac{t}{\tau_i}} + n_k(0) \frac{\tau_i}{\tau_k - \tau_i} e^{-\frac{t}{\tau_k}} \tag{2.4}$$

In the case of $\tau_k > \tau_i$

$$n_i(t) = n_i'(0) e^{-\frac{t}{\tau_i}} + n_k'(0) e^{-\frac{t}{\tau_k}} \tag{2.5}$$

where

$$n_i'(0) = n_i(0) - n_k(0) \frac{\tau_i}{\tau_k - \tau_i}, \quad n_k'(0) = n_k(0) \frac{\tau_i}{\tau_k - \tau_i} \tag{2.6}$$

and in the case of $\tau_k < \tau_i$

$$n_i(t) = n_k''(0) e^{-\frac{t}{\tau_i}} - n_k''(0) e^{-\frac{t}{\tau_k}} \tag{2.7}$$

$$n_k''(0) = n_i(0) - n_k(0) \frac{\tau_i}{\tau_i - \tau_k} \quad \text{and} \quad n_k''(0) = n_k(0) \frac{\tau_i}{\tau_i - \tau_k} \tag{2.8}$$

Therefore in either case $n_i(t)$ can be expressed as sum of two exponentials.

Similarly in presence of $N-1$ cascades, $n_i(t)$ can be written as

$$n_i(t) = \sum_{i=1}^{N} n_i'(0) e^{-\frac{t}{\tau_i}} \tag{2.9}$$

and writing it in conventional notations

$$\bar{I} \equiv \sum_{i=1}^{N} C_i e^{-\alpha_i t} \tag{2.10}$$

Where $\bar{I}$ is the fitting intensity for certain transition, $C_i = n_i'(0)$ and $\alpha_i = 1/\tau_i$.

An atomic decay curve is usually a sum of many exponentials, however, in most of the cases one to three exponential fit gives a very good approximation of the primary lifetime. Many numerical methods are employed to multiexponential fit
of an experimental decay curve. The most frequently used technique is the method of least squares, which minimizes a quantity, $S^2$, defined as

$$S^2 = \sum_j \left[ \frac{I(t_i) - \bar{I}(C_1, C_2, \ldots ; \alpha_1, \alpha_2, \ldots, \alpha_n)}{\sigma_j} \right]^2$$  \hspace{1cm} (2.11)$$

where $I(t_i)$ is the intensity at channel $i$, $t_i$ is the centroid of the channel $i$, $\bar{I}$ is the fitted intensity as given in the equation (2.10) and $\sigma_j$ is the standard deviation in the measurement of $I(t_i)$. Estimated parameters of $C$’s $\alpha_i$’s, are provided as input data with proper sign to the least squared fit and minimization of $S^2$ determines the fitted set of $C$ and $\alpha$ parameters.

A more rigorous method for correcting the effects of cascade repopulation on beam-foil lifetime measurements is to incorporate the intensity decay data for the important cascades directly in the analysis of the data for the primary transition by means of ANDC (Arbitrary Normalized Decay Curves) technique [1]. The basic ANDC relation is

$$\int_1^{T_j} dI_{jk} = -\frac{1}{\tau_j} \int_1^{T_j} I_{jk}(t) dt + \sum_i \frac{S(j \rightarrow k)}{S(i \rightarrow k)} A_{jk} \int_1^{T_j} I_{ij}(t) dt$$  \hspace{1cm} (2.12)$$

Where $\tau_j$ is the lifetime of the level, $j$, observed via the transition $j \rightarrow k$, transition $i \rightarrow j$ are the direct cascades repopulating level, $j$ and $S(a \rightarrow b)$ is the relative sensitivity of the detection system at the wavelength of the transition $a \rightarrow b$.

The transition probability for the spontaneous decay processes, $A_{ij}$, for transition from state $j$ to $i$, can be calculated from the measured mean lifetime $\tau_j$, via the expression

$$A_{ij} = \frac{B_{ij}}{\tau_j}$$  \hspace{1cm} (2.13)$$

Where $B_{ij}$ is the branching ratio for the corresponding transition. Then the
absorption oscillator strength, $f_{ij}$, can be obtained from the expression

$$A_{ij} = \frac{8\pi^2 e^2}{m_e c^2} \frac{g_i f_{ij}}{g_j \lambda_{ij}^2} = 0.6672 \frac{g_i f_{ij}}{g_j \lambda_{ij}^2} \text{(sec}^{-1}) \quad (2.14)$$

Where $e$ is the electron charge, $m_e$ is the mass of an electron, $c$ is the velocity of light and $g_i$ and $g_j$ are the statistical weights.

**2.2. Forbidden Radiative Transitions**

A radiative transition is said to be forbidden if the allowed $E1$ process is prohibited by any one of the well known selection rule on $E1$ transition. If the state may still radiate, of course, via one of the weaker, forbidden decay channel such as $M1$ (magnetic dipole), $E2$ (electric quadrupole), $M2$ (magnetic quadrupole) or $2E1$ (two-photon electric dipole) for which the selection rules are less rigorous. The transition rates for all such processes are smaller than that for the allowed processes and are very difficult to measure for atoms or near neutral ions. As a heavy ion becomes more highly stripped, however, the forbidden decay rates, which scale strongly with $Z$, become appreciable and eventually even dominate over competing $E1$ decays. A state that can only radiate via forbidden processes is said to be metastable against radiation. Thus metastable states are long-lived for near neutral species but become short enough for beam–foil time of flight measurements in highly stripped, high–$Z$ ions. Most atoms and their isoelectronic ions have at least one metastable state but until now beam–foil studies have concentrated on metastability in one–, two– and three–electron ions [2,3].

All of the $1s2p \ ^3P_l$ levels can decay by $E1$ transitions to the $1s2s \ ^3S_1$ level, an intrashell process that scales as $Z$ in the limit of large $Z$. A competing decay mode for the depopulation of the $1s2p \ ^3P_l$ level is the spin–forbidden (intercombination or intermultiplet) transition to the $1s^2 \ ^1S_0$ ground state. For ions with $Z \geq 6$, this spin forbidden process dominates the $E1$ decay channel to the
The beam foil results, for example, of Sellin et al [4,5] (Z=7,8), Mowat et al [6] (Z=9), Richard et al [7](Z=9) and Varghese et al [8] (Z=14,16) are all in essential agreement with theoretical predictions for this transition. The 1s2p 3P_2 level has a spin–forbidden (intermultiplet) M2 decay channel to the ground state which also competes with the allowed E1 decay to the 1s2s 3S_1 level. The rate for this M2 process scales as $Z^8$ and so eventually (Z≥17) it dominates the intrashell E1 process. There are no possible E1 transitions out of the 1s2s 1S_0 or the 1s2s 3S_1 levels. The 1s2s 1S_0 cannot decay by any single-photon process due to the rigorous selection rules on J(0–0). A two-photon decay process is possible (2E1) and this gives rise to continuum emission. Rate: for the 2E1 process, which scale as $Z^4$, becomes sufficiently rapid for high Z–ions that shows continuum, is observable in beam–foil experiments. For example, Marrus and Schmieder [9] studied this continuum using coincidence techniques in several ions including He–like argon. The 1s2s 3S_1 level can also radiate by a 2E1 process similar to that just described for the 1s2s 1S_0 level. However, it has also been quite recently established that a competing M1 transition, producing a discrete line, is also permitted. Relativistically induced M1 process scales as $\sim Z^{10}$ and it dominates the 2E1 process at high Z. An experimental confirmation for this type of transition was first made by Marrus and Schneider [10] in He–like silicon, sulfur and argon. Lifetime measurements on other highly stripped He–like ions were later made by Gould et al [11], Cocke et al [12] and Bednar et al [13]. At first, there appeared to be a discrepancy between the experimental measurements and the theory of Drake [14] and Johnson and Lin [15]. Later, however, it was found that experimental results approached the theoretical values if measurements were made downstream from the foil at distances corresponding to more than one decay length of the 1s2s 3S_1 level. Transition probabilities for the spin–forbidden 1s²2s² 1S_0–1s²2s²p 3P transition in Be–like Fe and Kr have been measured by Dietrich et al [16]. In case of He–like ions, the state 1s2p 3P_2 can
Fig. 2.1. Level diagram and radiative decay modes of the n=2 states of He–like ions
The decay to the ground state 1s² ¹S₀ by a magnetic quadrupole transition M2. The probability of this transition is given by [40].

\[
M2:A(1s^2 ¹S_0 \rightarrow 1s2p ³P_2) = \frac{a^7 Z^8}{1215} \left[ 1 + 0.28(aZ)^2 \right] \frac{me^4}{\hbar^3} \left( \frac{\Delta E}{Z^2 \text{Ry}} \right)^5
\]

\[
= 0.037Z^8 \left[ 1 + 0.28(\beta Z)^2 \right] \left( \frac{\Delta E}{Z^2 \text{Ry}} \right)^5 \text{[see}^{-1}] \tag{2.15}
\]

The comparison of Eq. (2.15) with numerical calculations tabulated in [17] shows that for Z>30 it is accurate to within 10–15%.

The decay mode to the excited state 1s2s ³S₁ for Z<18 is more effective than the M2 decay mode to the ground state. But for large Z, the M2 decay 1s² ¹S₀ \rightarrow 1s2p ³P₂ dominates. The level diagram and radiative decay modes of the n=2 states of He-like ions is shown in Fig. 2.1.

### 2.3. Forbidden Auger Transitions

The 1s2s2p ⁴P₃/₂ level of the lithium sequence is particularly interesting since being the lowest lying quartet level it is metastable against both radiation and Auger emission. The UTORNL group has measured [18] the lifetime of this metastable level in lithium ions of oxygen, fluorine, silicon, sulphur, chlorine and argon. This incidentally is a good example of how the beam-foil method can be used to study many different members of the isoelectronic sequence. Groeneveld et al [19] have made similar measurements in Li-like nitrogen, oxygen and neon and Bruch et al [20] have reported measurements on near neutral Li-like ions. The 1s2s2p ⁴P₃/₂ level has two primary de-excitation channels both of which are forbidden but which scale quite differently with Z. Thus the level can relax via an Auger process (autoionization) induced by the tensor part of the spin–spin interaction between the electrons, a process that appears to scale as \( Z^{3/2} \). Radiative de-excitation of this level via a spin–forbidden M2 transition to the ground state has also been observed [21,22] and this process scales as \( Z^5 \) for large
Following the suggestion by Cocke et al [21] that the rate for this M2 process in Li–like ions would be approximately equal to the known rates for the analogous transition He–like ions. Pegg et al [23] estimated from the lifetime results that the fluorescence yield (branching ratio for the M2 radiative process) was less than 1% for Li–like ions with Z≤10. This yield increases, however, to ~20% for Z=17. The estimates were later confirmed and extended by the Dirac–Hartree–Fock calculations of Cheng et al [24] who were the first to calculate the transition rates for both the Auger and radiative channels.

2.4. Satellites of Spectral Lines

The spectra of multicharged ions are much richer as compared to those of neutrals because of the presence of so called satellite lines arising from the radiation decay of autoionizing states where two or more electrons are excited, such states lie above the ionization limit and are created by either direct excitation of the inner shell electron or by capture of a free electron. It is essential for all satellite lines that the upper level is always an autoionizing one, i.e. it lies above the first ionization limit, while the lower level may be associated either the ground state or with one of the excited states as shown in the Fig. 2.2. The intensity of the satellite increases as the ion charge increases. Li–like autoionizing state can be produced by a capture of a free electron

\[ X_z(a_0) + e \rightarrow X_{z-1}^*(y) \]  

(2.16)

The radiative decay of an ion Eq. (2.16) leads to the dielectronic recombination process

\[ X_{z-1}^*(y) \rightarrow X_{z-1}^*(y) + \hbar \omega \]  

(2.17)

Let \( a_i \) denote the set of quantum number of an ion \( X_z \) in the initial state. The satellite transition \( a_i \rightarrow a_0 \) is called the line corresponding to transition \( a_0nl \rightarrow a_i nl \) of an ion \( X_{z-1} \), where \( n l \) are the quantum
Fig. 2.2. The origin of the satellite in H– to Li–like Ions
numbers. For example, $1s^2 \text{nl} - 1s2p\text{nl}$ transitions in Li-like ions are the satellites to the resonance line in He-like ions $1s^2 - 1s2p$. The lines arising in dielectronic recombination Eq. (2.17) are called the dielectronic satellites. In highly charged ions, the wavelength of satellites are very close to the "parent" line and their intensities increase with increasing $Z$.

2.5. Theoretical Descriptions

2.5.1 Introduction

As far as the theoretical situation in atomic physics is concerned, almost all the theories are based on independent particle approximation (IPA). Since ions or atoms with more than one electron are many body systems, the IPA model cannot describe the atomic behaviors of atoms of high atomic number. It does not explain many body effects like giant dipole resonance (GDR) in atoms [25]. As electrons do not remain dynamically independent in presence of spin–orbit interaction, the electron correlation effects become important [25]. However, the calculations taking electron–electron correlation through proper choice of interaction inside self consistent field (SCF) scheme become formidable. Relativistic correction (order of $\alpha^2$ and higher order terms) to atomic data is undoubtedly very important for heavy atoms and for inner shell electrons of any atoms. Even it has considerable effect on outer shell electrons since relativistic effect on energetic inner shell orbits changes the potential in which less energetic outer shell electrons move [26]. As a consequence, even though outer shell electrons are generally non–relativistic, their energies are affected by the relativistic effects. For the interpretation of the experimental results, many theoretical results are often called upon. Hence we will briefly discuss a few important theories such as relativistic random phase approximation (RRPA) [27,28], multi configuration Hartree–Fock with relativistic effects included using either Breit–Pauli interaction or simple parameterized spin–orbit interactions.
multiconfiguration Dirac–Fock (MCDF) calculation, Dirac–Hartree–Slater calculation, used extensively to interpret some of our results. We make use of Hartree atomic units unless otherwise indicated (\( e = \frac{\hbar}{2\pi} = m_e = 1 \)), whence \( c = 1/\alpha; \) \( e \) is charge of the proton, \( h \) is the Planck’s constant, \( m_e \) is the mass of the electron, \( c \) is the speed of the light in vacuum and \( \alpha = 1/137.0359895 \) is the fine structure constant.

### 2.5.2. Multiconfiguration Hartree–Fock Calculation

The abinitio theories which are based on independent particle approximations (self–consistent field method) and variation methods, Hartree–Fock formalism is the historical one. Configuration interaction with a fixed core has been included into it which is known as multiconfiguration Hartree–Fock method. Obviously, solutions of many electron systems using this method can only be possible numerically. Main features of such calculations are sketched below, as described in the reference [32]. The nonrelativistic Hartree–Fock Hamiltonian, in atomic units, is given by

\[
H = -\frac{1}{2} \sum_{i=1}^{N} \left( \Delta_i^2 + \frac{2Z}{r_i} \right) + \sum_{i>j} \frac{1}{R_{ij}} \tag{2.18}
\]

Where \( Z \) is the atomic number and \( R_{ij} = |\vec{r}_i - \vec{r}_j| \) is the distance between ith and jth electron. This expression assumes the nucleus can be treated as a point charge with infinite mass. The multiconfiguration Hartree–Fock approach is similar to the MCDF calculation which will be discussed in the next section. The Hartree–Fock wave function for an atomic state is

\[
(\Gamma LS) = \sum_{\nu} c_\nu \phi(\gamma, LS), \quad \sum_{\nu} c_\nu^2 = 1 \quad \text{and} \quad <\phi(\gamma_0, LS) | \phi(\gamma_k, LS)> = \delta_{\nu_0} \tag{2.19}
\]
where $\phi(\gamma_{LS})$ is the configuration state function, an analogue of $|\Gamma_J \Omega M \rangle$ in MCDF formalism which is an antisymmetric function known as the "Slater determinant" for a set of spin–orbitals $\Phi_p(i)$, an orbital for the pth set of quantum numbers in terms of space and spin coordinates of the ith electron

$$\left[-\frac{1}{2} \Delta_i + \frac{2Z}{r_i} + V(r_i)\right] \phi_p(i) = E_i \phi_p(i) \quad (2.20)$$

is the single particle potential (a combination of direct and exchange contributions of electron–electron coulomb interaction) and

$$V(r_i) = \frac{1}{2} \int \phi_p(i) \phi_q(j) \frac{1}{R_{ij}} \phi_p(i) \phi_q(j) dr_i - \frac{1}{2} \int \phi_p(i) \phi_q(j) \frac{1}{R_{ij}} \phi_q(i) \phi_p(j) dr_i \quad (2.21)$$

is the single particle potential (a combination of direct and exchange contributions of electron–electron coulomb interaction) and

$$\phi_{nlm\sigma}(r, \theta, \phi, \sigma) = \frac{1}{r} P(nl;r) Y_{nlm}(\theta, \phi) \chi_{m\sigma} \quad (2.22)$$

where $Y_{nlm}(\theta, \phi)$ is the spherical harmonic and $\chi_{m\sigma}$ is a spin function. The radial function $P(nl;r)$ is now a solution of the radial Schrödinger equation

$$\left\{ \frac{d^2}{dr^2} + \frac{2Z}{r} - 2V(r) - \frac{l(l+1)}{r^2} + 2E - i \right\} P(nl;r) = 0 \quad (2.23)$$

The above equation satisfies the boundary condition $P(0) = P(\infty) = 0$

To determine $\psi(\Gamma_{LS})$ both the radial functions $P(nl;r)$ and the mixing coefficient $c_i$ are determined variationally. $\psi(\Gamma_{LS})$ is used further to calculate relativistic effects in ion and atom through Breit–Pauli approximation where the Hamiltonian is expressed as a sum of the nonrelativistic Hamiltonian (2.18) and the relativistic correction ($H_R$). The relativistic correction is made by perturbative approach.

$$H_{BP} = H + H_R \quad (2.24)$$

where $H_R$ is a sum of the following contributions: the one-electron spin–orbit
interaction, the relativistic mass correction, the one body Darwin term the spin–
other–orbit interaction, the dipolar spin–spin interaction, the orbit–orbit
interaction, the two body Darwin term and the spin–spin contact term. This
approach called is MCHF+BP. Since MCHF+BP methods is very much
computer time consuming, sometimes spin–dependent part of the Hamiltonian
i.e., is accounted in the simpler form as given below

\[ H_{so} = \sum_{i=0}^{n} \frac{\tau_i}{r_i^3} l_i s_i \]  

(2.25)

where \( \tau_i \) is a parameter, dependent on the \( l \)-value of the electron involved in the
interaction which can be chosen to give the best fit to experimental values of the
fine structure splitting of appropriate states.

2.5.3. Multiconfiguration Dirac–Fock Calculation

As for example, even in case of hydrogen, the Lamb shift is due to
relativistic effects [33]. Relativistic effect of a light ion can be important if more
than one electron behave as valance electrons [34]. In particular for heavy ions
and atoms, relativistic effects and effects produced by the interaction between
electrons are strongly interwined. Therefore, relativity and electron correction
should be accounted on an equal footing: neither will be considered simply a
perturbation to the other.

All these considerations are incorporated in multiconfiguration Dirac–Fock
calculations. These calculation for many electron system are not, obviously, an
analytically solvable. A number of computer programs are presently available.

Relativistic atomic orbitals are one–electron spin or eigenfunctions of
parity, \( \pi \), and angular momentum \( \hat{j}^2, \hat{j}_z \). Configuration state functions (CSFs)
are built from antisymmetrized products of such orbitals and have prescribed
coupling scheme, parity \( \Pi \), angular momentum \( J \) and \( M \) quantum numbers.
Multiconfiguration atomic state functions (ASFs) are linear combination of CSFs having common value of \( \Pi, J \) and \( M \) quantum numbers. Multiconfiguration atomic state functions (ASFs) are linear combination of CSFs having common value of \( \Pi, J, \) and \( M \). Matrix elements of Hamiltonian etc., between CSFs are calculated using Racah algebra. Finite-difference methods are used in all operations on radial functions. Radial wave functions of great variety can be generated by the program. MCDF predictions have been used throughout the work in the thesis.

2.5.4. Dirac–Hartree–Fock (DHF) Calculation

The basic one-electron states are constructed from solutions to the Dirac equation including the ground-state Dirac–Hartree–Fock potential. DHF potential takes into account the principle effect of the electron–electron interaction together with the nuclear Coulomb field and the ground-state self-consistent potential in the field operator \( \psi \) by expanding \( \psi \) in the complete set of solutions to the Dirac equation. DHF calculations can be utilized for both radiative as well as autoionizing decay thus lifetime of \( 1s2s2p \, {}^4P_{5/2} \) can be estimated with this method.

The radiative M2 decay rate of the \( 1s2s2p \, {}^4P_{5/2} \) state is written as

\[
w(M2) = \frac{12}{5} \alpha E |M(E)|^2
\]

(2.26)

where \( \alpha \) is the fine structure constant, \( E \) is the photon energy and \( M(E) \) is the matrix element as given in the [24].

The autoionization rate is determined to be

\[
w(auto) = \frac{16}{5} \alpha^2 pE \left| \frac{1}{3} R_1 - \frac{1}{5} R_2 \right|^2
\]

(2.27)

where \( p \) and \( E \) are the momentum and energy of the continuum \( f_{5/2} \) electron and...
\( R_1 \) and \( R_2 \) are the magnetic Slater integrals as given in the [24]. So the lifetime can be calculated as

\[
\tau = \frac{1}{w(M2) + w(auto)}
\]

(2.28)

The results of Dirac–Hartree–Fock (DHF) calculations of the M2 radiative decay rates for elements of Li–isoelectronic sequence in the range \( Z=3 \) to 26 [24] was good in agreement with experimental results. We have compared the results of the experiment with theory. It was a good agreement.

2.5.5. Relativistic Random Phase Approximation

A relativistic version of the random phase approximation (RPA) is used to study allowed and forbidden radiative transition in atoms. The theory is applied to the He isoelectronic sequence to test its utility. Theoretically determined data, moreover, can now be subjected to scrutiny in the laboratory using beam–foil spectroscopy [35].

For atomic transitions in highly stripped ions relativistic effects become more and more important as the nuclear charge \( Z \) of the species increases. It seems desirable to develop a theory of atomic transitions for high \( Z \)- atoms which includes relativistic effects nonperturbatively. Relativistic theories which do not account for correlations, however, are likely to be unreliable. The traditional configuration–interaction method used to treat correlation's in the nonrelativistic theory appears to present computational difficulties in the relativistic case. Therefore, in view of the successes and simplicity in nonrelativistic theory, Johnson and Lin [28] have introduced a relativistic version of the random phase approximation (RPA) to treat those correlation effects which are important in the calculation of radiative transitions in closed shell atoms [36].

The random phase approximation (RPA) was originally developed to study extended systems such as electron gases or nuclear matter [37]. It has been
applied to a wide class of atomic and molecular processes, especially for the
computation of transition probabilities and photoionization cross sections [38].
The RPA leads to a treatment of correlations in which the computational
advantages of an independent–particle theory are retained. From a physical point
of view correlation effects in the initial and final states are treated simultaneously,
leading to oscillator strengths which satisfy the Thomas–Reiche–Kuhn sum rule
and which have identical values in the length and velocity forms.

In the nonrelativistic theory the RPA provides a generalization of the
Hartree–Fock (HF) equations. The difference between the RPA and HF theory is
due to the certain correlation effects. A valuable consequence of the relativistic
approach is that forbidden transitions are obtained with the same case as allowed
transition.

The nonrelativistic RPA takes three equivalent forms [39] as applied by
different workers, namely time–dependent Hartree–Fock (TDHF) theory [40],
the linearized equations–of motion method [41] and the Green’s function method
[42].

The formulation of the theory and a discussion of the numerical methods
used to solve the relativistic RPA equation is given in the reference
Johanson and Lin [28]. Precise numerical solutions to the relativistic RPA
equations are obtained describing the transitions $1s^2 \ 1S_0 - 1s2s \ 3S_1$ (M1),
$1s^2 \ 1S_0 - 1s2p \ 3P_1$ (E1) and $1s^2 \ 1S_0 - 1s2p \ 3P_2$ (M2). The resulting excitation energies
and transition probabilities are in good agreement with accurate nonrelativistic
calculations for low Z elements. For intermediate and high Z elements where
relativistic effects are more important, the results are expected to be very
accurate. The results obtained in case of metastable states have been compared
with our experimental results as shown in the chapter 4 and 5.

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References


