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**INTERNATIONAL CENTRE FOR
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**LAMP
SERIES REPORT**

(Laser, Atomic and Molecular Physics)

**THE EFFECTS OF CORRELATION, RELATIVITY, QUANTUM
ELECTRODYNAMIC, NUCLEAR SIZE AND PARITY
NON-CONSERVATION IN ALKALI ATOMS
AND ALKALI-LIKE IONS**

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**INTERNATIONAL
ATOMIC ENERGY
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**UNITED NATIONS
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ORGANIZATION**

MIRAMARE-TRIESTE

International Atomic Energy Agency
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Preface

The ICTP-LAMP reports consist of manuscripts relevant to seminars and discussions held at ICTP in the field of Laser, Atomic and Molecular Physics (LAMP).

These reports aim at informing LAMP researchers on the activity carried out at ICTP in their field of interest, with the specific purpose of stimulating scientific contacts and collaboration of physicists from Third World Countries.

If you are interested in receiving additional information on the Laser and Optical Fibre activities at ICTP, kindly contact Professor Gallieno Denardo, ICTP.

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ABSTRACT

The present review briefly presents the growing experimental as well as theoretical interests in recent years in the effects of (1) correlation, (2) relativity, (3) quantum electrodynamic (QED), (4) finite nuclear size (FNS) and (5) parity non-conservation (PNC) on the high precision electronic structure of alkali atoms and alkali-like ions. Many high precision experiments have been performed which need very high accurate theoretical prediction for correct interpretation and identification of different physical effects involved. Some experiments separate these effects and some do not. Several sophisticated theoretical techniques have been developed for corrections of these effects which play an extremely important role in order to obtain results of high accuracy to well below 1% level and to understand experimental observations of high precision. Correlation, relativity and finite nuclear size effects have been treated on an equal footing in some theoretical methods but QED and PNC have been calculated separately. At present, there is no theory which accounts all five effects in a coherent and unified manner. Future challenges and directions, in reliable structure calculations in atoms and ions, have been discussed and suggested.

1 Introduction

There has been growing interest in alkali atoms and alkali-like ions for both experimentalists as well as theorists, partly because of their simple electronic structure, with only one valence electron outside energetically separated inner cores. Most of these investigations concern the various spectroscopic energies. Knowledge of wave functions which reproduce closely the observed spectra of the atoms is required for calculating other properties, such as oscillator strengths and life times, magnetic moment, or the magnetic field generated at the nucleus by the valence electron charge flow. Recent high precision experiments measuring parity non-conservation in heavy alkali atoms such as Cs have shown that atomic experiments are competitive in investigating weak interaction between elementary particles. Atomic calculations of very high accuracy are necessary to obtain information about weak interaction. The accuracy of computational methods may be assessed by the quality of the level energies they predict. A number of theoretical models have been developed to describe the properties of atoms, molecules and ions.

Independent particle models (e.g. central potential model, Hartree-Fock Slater method, Hartree-Fock method) describe qualitatively the properties of many-electron atoms, molecules and ions. Independent particle model deviates quantitatively substantially from the experimental observations. It clearly demonstrates that it is indispensable to incorporate electron correlation in order to obtain accurate results. Electron correlation is defined as the difference between the exact energy for a certain Hamiltonian and the Hartree-Fock (or single configuration) energy for the same Hamiltonian operator. It is simply the correction to zero-order approach. A physical

interpretation is the dynamic behaviour of the electrons, which in single configuration model move independently of each other in an average central field. Correlation introduces the fact that they actually do avoid each other in their orbits. Nonrelativistic correlations are included widely in two methods: configuration-interaction (CI) and multiconfiguration Hartree-Fock (MCHF). Tiwary and his *co-workers*¹⁻³¹ have extensively investigated the effect of correlation on the optical oscillator strengths, both the length (f_L) and velocity (f_V) forms, in alkali atoms and alkali-like ions using uncorrelated and correlated wave functions for both the initial and final states involved in the transition. For ground state configuration, all orbitals are taken from Clementi and Roetti³². Several standard computer codes³³⁻⁴⁰ are available for the accurate atomic structure calculations. For low Z atoms and ions, these methods produce good results but for heavy systems they disagree with the experiment which suggest that relativistic as well as correlation effects play important role for reliable results.

Accurate prediction of excitation energies, oscillator strengths, lifetime, etc., in alkali atoms and alkali-like ions, particularly for the heavier members of the group, requires high-order incorporation of both relativistic and correlation effects. We therefore start from the Dirac⁴¹ Coulomb or Dirac-Coulomb-Breit⁴² Hamiltonian. The latter is correct to the second order in the fine structure constant. The four-component one-electron equations, in the Dirac-Fock or Dirac-Fock-Breit approximation, are solved. Relativistic correlation is then incorporated by the multiconfiguration Dirac-Fock (MCDF) method.

Relativistic and electron correlation effects are strongly intertwined. Accurate treatment of many electron systems requires therefore going beyond the independent particle model to incorporate relativistic and correlation simul-

taneously on an equal footing. A variety of techniques can be employed for the study of dynamic correlation in particle systems. The extensive practice of nonrelativistic as well as relativistic calculations, including those for alkali atoms shows that many body perturbation theory is a powerful and systematic approach. The first few terms of the perturbation series suffice for accurate calculations of the properties of highly charged ions, but the method is less suitable for neutral atoms, where higher orders of MBPT are non-negligible and sometimes even make the convenience of the perturbation expansion doubtful. The expression for higher order terms are complicated and direct perturbative studies are rarely carried out beyond second order wave functions or third order energies. It is clearly desirable to explore methods which identify important physical effects and incorporate them to all orders in perturbation theory.

One of the most interesting features of the developments of physics is when an established and successful theory is shown to be only an approximation to reality and a deeper and more encompassing theory replaces it. This has happened many times in physics: Newton theory of gravitation was replaced by Einstein general theory of relativity, nonrelativistic mechanics with relativistic mechanics, nonrelativistic classical mechanics with nonrelativistic quantum mechanics and so on. In each case the older theories remain of value but they are recognized to be only in their domain of validity. Very frequently precise measurements play a significant role in replacing a theory with a deeper or covering theory. Another exciting example is about 46 years ago when the Dirac theory⁴¹ of hydrogen, which predicted the exact degeneracy of the $2 S_{1/2}$ and $2 P_{1/2}$ states, was shown to be very slightly incorrect by the measurement of the Lamb shift⁴³. As tiny as the effect is,

it requires the complete replacement of Dirac relativistic generalization of the Schroedinger equation. In order to explain the Lamb shift, a relativistic quantum field theory of the interacting electrons and electromagnetic fields was developed in the form of Quantum Electrodynamics (*QED*)^{44–65}.

The *QED* has widely applied to interpret several experimental observations of high precision. There are several theories available in the literature. All are approximate. There are main two parts of *QED*: self energy and vacuum polarization. We concentrate on *QED* effect in Li-like U^{89+} ion.

High precision experiments exhibit that only correlation, relativity and *QED* effects are not able to explain measurements. The effect of finite nuclear size (*FNS*)^{66–72}, though extremely small, was incorporated to interpret accurate observations. Several theoretical calculations are available for the *FNS* correction in atoms, molecules and ions. Recently, very high precision atomic experiments have demonstrated that the inclusion of only correlation, relativity, *QED* and *FNS* are not adequate to interpret accurate observations. The parity nonconservation (*PNC*) effect must be incorporated in order to explain measurements.

The parity of a system describes its behaviour under reflection through the origin. This transformation is formally equivalent to a mirror reflection in a plane through the origin plus a 180° rotation about an axis perpendicular to that plane. Rotational invariance of physical system means that a parity non-conserving (*PNC*) system is one that exhibits a mirror asymmetry. Of the four fundamental interactions, only weak interaction is known to be parity non-conserving. The effects of weak interaction in the atomic environment leads to small mirror asymmetry such as the rotation of plane

polarized light in an atomic vapour. These effects, though extremely small, are measurable because of their *PNC* signature. Advances in experimental techniques have enabled high precision measurement of atomic *PNC* phenomena. Atomic *PNC* effects have a Z^3 enhancement so that experiments are performed on heavy atoms: currently, atomic *PNC* experiments have been performed on Cs, Tl, Pb and Bi.

During the past decade, experiments to detect atomic *PNC* have progressed to a point where *PNC* amplitude can be measured with an accuracy of a few percent. To interpret such experiments in terms of the standard model of the electro-weak interaction, it is necessary to compare the measured amplitude with theoretically predicted amplitude. Predicted *PNC* amplitudes in heavy atoms to a accuracy of one percent is challenging exercise in many-body theory that leads beyond the independent particle model and low order perturbation theory to techniques in which important terms in perturbation theory are summed to all orders. The most precise experiments and theory have been made for Cs because the requisite atomic structure calculations can be carried out for the cesium than for the other elements.

The principal source of *PNC* in atoms is the exchange of Z_0 bosons between bound electrons and the atomic nucleus. The *PNC* interaction from Z_0 exchange consists of two parts: a dominant part in which the vector nucleon current is coupled to the axial vector electron current and a much smaller part in which the axial vector nucleon current is coupled to the vector electron current. The parity conserving part of the Z_0 exchange interaction is, of course, masked by the electron-nucleus Coulomb interaction.

Usually physicists consider measurements of the effects of *PNC* as a method to investigate the strength and structure of weak interaction. However, there is one other possibility i.e. investigation of a complicated quantum system or process using the *PNC* effects as a probe. These effects are always linear in

the weak interaction matrix elements and provide more detailed information than level spacings, widths, etc. A wide range of physical effects is involved in the study of *PNC*⁷³⁻⁸³ which makes it a stimulating and rewarding field. Using PNC effects one can study quantum chaos, phase transitions, nuclear fission, distribution of neutrons in nuclei, properties of weak interaction, the accuracy of both calculation and measurement to well below 1 % level, etc.

2 Theory

2.1 Correlation

Very general methods, that take into account of nonrelativistic correlation and can be used for even the most complex atoms and ions, are the configuration interaction (CI) and multiconfiguration Hartree-Fock (MCHF), which are closely related.

The basic assumption of both sets of methods is that the atom or ion is represented by an atomic or ionic state function (ASF or ISF), $\Psi(LS)$, which is a linear combination of configuration state functions (CSF), $\Phi(\alpha_i LS)$. The LS wave functions are written in the form:

$$\Psi(LS) = \sum_{i=1}^{NCSF} c_i \Phi_i(\alpha_i LS) \quad (1)$$

Each CSF is constructed as a coupled, antisymmetric sum of products of one particle functions, $\phi_{nl}(\tau)$, called spin-orbitals,

$$\Phi_{nl}(\tau) = \frac{1}{r} P_{nl}(\tau) Y_{m_l}^l(\theta, \varphi) \chi_m, \quad (2)$$

The coefficients c_i are the eigenvectors components of the Hamiltonian matrix with typical element

$$H_{ij} = \langle \Phi_i | H | \Phi_j \rangle \quad (3)$$

Φ_j are single-configuration functions constructed from one-electron functions, whose orbital and spin momenta are coupled to form the common total angular-momentum quantum numbers L and S according to a prescription denoted in (1) by α_i .

We express the radial parts of the one-electron functions in analytical form as a sum of Slater-type orbitals, following Clementi and Roetti³² :

$$P_{nl} = \sum_{j=1}^k C_{jnl} r^{l_j n_l} e^{-\xi_{jnl} r} \quad (4)$$

The parameters in (3) can be varied to optimize the energy of any state, subject to the orthonormality conditions

$$\int_0^\infty P_{nl}(\tau) P_{n'l'}(\tau) d\tau = \delta_{nn'} \quad (5)$$

In equation (1) and (2), there are two sets of unknown, the c_i coefficients and radial functions $P_{nl}(\tau)$. The difference between the CI and MCHF methods is now basically just the way the last set is obtained. In MCHF method, the variational principle is employed to derive a set of coupled integro-differential equations, one for each radial functions, while coefficients are obtained by solving a secular equation, of the form

$$[H - EI]c = 0 \quad (6)$$

where the matrix \mathbf{H} has the elements $H_{ij} = \langle \Phi_i | H | \Phi_j \rangle$ and H is the Hamiltonian operator. These two optimizations are performed at the same

time, in an iterative method usually labeled self-consistent field. In CI calculations, on the other hand, the radial functions are predetermined and only the secular equation is solved for the coefficients.

Once the radial wave functions are determined, relativistic effects may be added to the Hamiltonian in the form of the Breit-Pauli interaction, of which we include the spin-orbit, spin-other-spin, spin-spin, mass correction, and one-body Darwin terms. The Breit-Pauli Hamiltonian can be written as:

$$H^{BP} = H_{s-o} + H_{s-o-s} + H_{s-o-s} + H_m + H_{D1} \quad (7)$$

The first three terms split LS states into J-dependent levels while the last two affect the overall energy of each term. The expansion (1) is then replaced by

$$\Psi(J) = \sum_i c_i \Phi_i(LSJ) \quad (8)$$

where the summation now includes single-configuration with different L and S (which can couple to form a common J value). The matrix which is diagonalized to give the eigenenergies and eigenvectors components a_i now contain the Breit-Pauli operators as well as the previous non-relativistic terms in the Hamiltonian.

2.2 Relativity

Many-electron Schroedinger Hamiltonian can be written as

$$H^S = \sum_{i=1}^N \left[\frac{p_i^2}{2m} - \frac{Z(\tau)}{r_i} \right] + \sum_{i \neq j} \frac{1}{|r_i - r_j|} \quad (9)$$

This Hamiltonian does not include the relativistic effect. In 1928, *Dirac*⁴¹ proposed a relativistic (Lorentz covariant) equation for an electron which, in the central field of a nucleus with charge Z, can be written as follows (in atomic unit):

$$H^D \psi = E \psi \quad (10)$$

where the Dirac Hamiltonian, H^D , is of the form (for one-electron system):

$$H^D = c\alpha \cdot p + c^2 \beta m - Z/r, \quad (11)$$

where

α is the Dirac matrix

$$\alpha = \begin{pmatrix} 0 & \sigma^P \\ \sigma^P & 0 \end{pmatrix} \quad (12)$$

and

β is the Dirac matrix

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad (13)$$

In equation (11) c is the velocity of light, r is the electron-nucleus distance (point nucleus is used, although the finite size of the nucleus presents no difficulties) and p is the linear momentum operator of the electron. The α and β are the Dirac 4×4 matrices, which can be written in the standard representation in terms of 2×2 Pauli matrices, σ^P , and 2×2 unit matrix, I as in equation (12,13).

The eigenfunctions, ψ , of equation (10) are four-component spinors and these can be chosen as eigenfunctions of the set of commuting operators: H^D , J^2 ,

the total angular momentum squared, J^2 , the projection of J on the Z-axis. The eigenvalues of these commuting operators are E , $j(j+1)$, m and k , respectively. The four-component eigen-spinors, ψ_{nkml} , can be written as:

$$\psi_{nkml}(r, \theta, \phi) = \begin{pmatrix} r^{-1}P_{nk}(r)\chi_{km}(\theta, \phi) \\ ir^{-1}Q_{nk}(r)\chi_{-km}(\theta, \phi) \end{pmatrix} \quad (14)$$

The $r^{-1}P_{nk}$ and $r^{-1}Q_{nk}$ are the large and small radial functions and the $\chi_{km}(\theta, \phi)$, the two-component spinors. Details are given elsewhere. It is well known that Dirac theory accounts for many experimental results for one-electron system. One may, therefore, believe that the Dirac theory is the starting point for a relativistic treatment of many-electron systems and the Dirac-Coulomb Hamiltonian for many-electron system can be written as

$$H^{DC} = H^D + H^C \quad (15)$$

$$H^{DC} = \sum_{i=1}^N [\alpha_i \cdot p_i + \beta_i m - \frac{Z(r)}{r_i}] + \quad (16)$$

$$\sum_{i \neq j} \frac{1}{|r_i - r_j|} \quad (17)$$

It is not possible to generalize the Dirac theory to many-electron systems. A fully Lorentz invariant Hamiltonian for many-electron systems can not be obtained in a closed form because the complete electron-electron interaction involves, in addition to the instantaneous Coulomb interaction (r_{ij}^{-1} which is not Lorentz invariant), the exchange of virtual photons between interacting electrons. However, *Breit*⁴² proposed H^{Br} as a correction to the Coulomb interaction, r_{ij}^{-1} for two electrons as:

$$H^{Br} = -\frac{1}{2} \left[\sum_{i=1}^N \frac{\alpha_i \cdot \alpha_j}{r_{ij}} + \frac{\alpha_i \cdot r_{ij} \cdot \alpha_j \cdot r_{ij}}{r_{ij}^3} \right] \quad (18)$$

The Dirac-Coulomb-Breit Hamiltonian H^{DCB} can be written as:

$$H^{DCB} = H^D + H^C + H^B \quad (19)$$

H^{Br} takes into account the magnetic and retardation terms and is of the order of $(Z/c)^2$, relative to the Coulomb interaction. Thus, it should be used as the first-order perturbation to the zeroth order Hamiltonian. The difficulty with this Hamiltonian is that the Breit interaction, which is a correlation to the nonrelativistic Coulomb interaction r_{ij}^{-1} , represents only the first order relativistic correlation. In the language of Feynman diagrams, it represents the exchange of only one virtual photon between the two interacting electrons. In principle, there are higher order corrections corresponding to the exchange of two, three, etc., virtual photons. Much work is still needed to calculate these higher-order corrections to the Breit interaction.

2.3. Basic Theory of Quantum Electrodynamics (QED)

Quantum electrodynamic corrections are the radiative corrections commonly known as the *Lamb Shift*⁴³. The Lamb shift may be written as a sum over terms representing different physical effects:

$$E_{LS} = \delta E_{SE} + \delta E_{VP} + \delta E_{FNS} + \delta E_{HO} + \delta E_{RC} \quad (20)$$

with: SE, electron self energy correction; VP, vacuum polarization correction; FNS, correction due to the finite nuclear size; HO, higher order corrections due to two virtual photons processes; RC, relativistic corrections (relativistic recoil and relativistic reduced mass).

From the point of view of field theory, the vacuum polarization correction is the result of the process in which the photon that mediates the Coulomb interaction between the bound electron and the nucleus produces a virtual electron-positron pair in the vacuum. The corresponding Feynman diagram

is given in figure 2. The diagram gives a corection to the Coulomb potential $V(r)$ known as the *Uehling*⁴⁵ potential $\delta V(r)$:

$$V(r) \rightarrow V(r) + \delta V(r) \quad (21)$$

In the Coulomb field of a nucleus of charge Ze , $\delta V(r)$ is given by

$$\delta V(r) = -\frac{\alpha}{\pi}(Z\alpha)f(r/\lambda_e)m_e c^2 \quad (22)$$

where

$$f(r/\lambda_e) = \frac{\lambda_e}{3r} \int_1^\infty dt (t^2 - 1)^{1/2} (2t^{-2} + t^{-4}) e^{-2tr/\lambda_e} \quad (23)$$

The range of the Uehling potential is exhibited by the asymptotic form for $r \gg \lambda_e$

$$f(r/\lambda_e) \sim -\frac{\pi^{1/2}}{4} \left(\frac{\lambda_e}{r}\right)^{5/2} e^{-\frac{2r}{\lambda_e}} \quad (24)$$

The range of δV is short on the atomic scale, so the energy shift is proportional to the bound electron wave function at the origin, to lowest order in $Z\alpha$:

$$\begin{aligned} \Delta E_U = \langle \delta V \rangle &= \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{n^3} G_n(Z\alpha) m_e c^2 \\ &\approx -\frac{\alpha}{\pi} (Z\alpha) |\psi(0)|^2 \int d^3r f(r/\lambda_e) m_e c^2 \end{aligned} \quad (25)$$

In (5), the function $G_n(Z\alpha)$ gives the exact expectation value of δV calculated with Dirac wave functions. For small Z , we have

$$G_n(Z\alpha) \sim \begin{cases} -\frac{4}{15} & s \text{ states} \\ 0 & p, d, \dots \text{ states} \end{cases} \quad (26)$$

The self energy is the dominant QED correction in ordinary atoms and ions. This is in contrast to muonic atoms where the vacuum polarization dominates. The first self energy calculation was done by *Bethe*⁴⁶ in 1947 based on the nonrelativistic formulation of radiation theory, including mass normalization. The expression he evaluated is :

$$\begin{aligned} \Delta E_{SE}^{Bethe} &= \frac{\alpha}{4\pi^2 c^2} \sum_{\lambda=1}^2 \int d^3k k^{-1} \langle n | \hat{\epsilon}_\lambda \cdot \vec{v} \sum_i \frac{|i\rangle \langle i|}{E_n - E_i - k} \hat{\epsilon}_\lambda \cdot \vec{v} | n \rangle \\ &\quad + \frac{1}{2} \delta m_0 \langle v^2 \rangle \end{aligned} \quad (27)$$

$$\Delta E_{SE}^2 = \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{n^3} F_n(Z\alpha) m_e c^2 \quad (28)$$

$F_n(Z)$ is approximately $4/3ln(Z\alpha)^{-2} + C_n$

$$H^{Furry} = \int d^3(r) \psi^\dagger(r) \left[\alpha \cdot p + \beta m - \frac{Z\alpha}{r} + U(r) \right] \psi(r) \quad (29)$$

$$\psi(x) = \sum_{n^+} b_n \phi_n(\vec{x}) e^{-iE_n t} + \sum_{n^-} d_n^* \phi_n(\vec{x}) e^{-iE_n t} \quad (30)$$

$$[-i\vec{\alpha} \cdot \vec{v} + V(\vec{x}) + \beta - E_n] \phi_n(\vec{x}) = 0 \quad (31)$$

The creation and destruction operators obey the usual Fermi anticommutation rules. Interaction of the electromagnetic current of the electron-positron field with the radiation field is provided by the interaction Hamiltonian density:

$$H_I(x) = -1/2e[\psi(x)\gamma^{m\mu}, \psi(x)]A_\mu(x) - 1/2\delta m[\psi(x), \psi(x)] \quad (32)$$

where $-e$ is the electron charge and A_μ is the vector potential of the radiation field. The second term in (12) is the mass renormalization counter term. Energy level shifts are calculated in a perturbation expansion in H_I by applying the Gell-Mann and Low theorems in the symmetric form discussed by Sucher

$$\Delta E_n = \lim_{\epsilon \rightarrow 0} \frac{i\epsilon}{2} \frac{\partial}{\partial \lambda} \frac{\langle n | S_{\epsilon, \lambda} | n \rangle}{\langle n | S_{\epsilon, \lambda} | n \rangle} \quad (33)$$

where

$$S_{\epsilon, \lambda} = \sum_{j=0}^{\infty} S_{\epsilon, \lambda}^j \quad (34)$$

and where

$$S_{\epsilon, \lambda}^j = \frac{(-i\lambda)^j}{j!} \int d^4x_j \dots \int d^4x_1 e^{\epsilon(|t_2| - \dots - |t_1|)} \times T[H_I(x_j) \dots H_I(x_1)] \quad (35)$$

$$|n\rangle = \sum_{i_1 \dots i_k} c_{i_1} \dots c_{i_k} b_{i_1}^* \dots b_{i_k}^* |0\rangle \quad (36)$$

$$S_F(x_2, x_1) = \begin{cases} \sum_{n^+} \phi_n(\vec{x}_2) \phi_n(\vec{x}_1) e^{-iE_n(t_2 - t_1)} & t_2 > t_1 \\ -\sum_{n^-} \phi_n(\vec{x}_2) \phi_n(\vec{x}_1) e^{-iE_n(t_2 - t_1)} & t_2 < t_1 \end{cases} \quad (37)$$

or

$$S_F(x_2, x_1) = \frac{1}{2\pi i} \int_{C_F} dz \sum_n \frac{\phi_n(\vec{x}_2) \phi_n(\vec{x}_1)}{E_n - z} e^{-iz(t_2 - t_1)} \quad (38)$$

Where C_F denotes the *Feynman*⁵² contour. The lowest order diagrams for the QED correction to the energy level are shown in Fig. 3.

Wichmann and *Kroll*⁵⁰⁻⁵¹ have examined the complete vacuum polarization

and have shown that the effect of correction to the Uehling potential included in the exact result is very small in ordinary atoms over a wide range of Z . In muonic atoms, on the other hand, this correction is of measurable magnitude.

2.4. Finite Nuclear Size (FNS)

Although, the nucleus is frequently taken to be a point source for an electron field, whence

$$V_{nucl} = -\frac{Ze^2}{r} \quad (39)$$

is the potential energy of interaction between an electron and nucleus, other models the account for the finite size of the nuclear charge distribution are commonly employed for high precision calculations and

$$V_{nucl} = -\frac{Z(r)\epsilon^2}{r} \quad (40)$$

Possible models for the charge distribution in the nucleus include a hollow shell charge distribution with radius R_s ,

$$\rho_s(r) = \frac{Ze}{4\pi R_s^2} \delta(r - R_s), \quad (41)$$

a spherically symmetric uniform charge distribution with surface radius R_u

$$\rho_u(r) = \frac{Ze}{4/3\pi R_u^3} \theta(R_u - r), \quad (42)$$

and the Fermi model

$$\rho_f(r) = \frac{\rho_0}{1 + e^{\frac{r-a}{\alpha}}}. \quad (43)$$

For the binding energy, the dependence on the model is small provided the root mean square (rms) radius of the charge distribution

$$R = \left[\frac{1}{Ze} \int dr r^2 \rho(r) \right]^{1/2} \quad (44)$$

is fixed to a particular value.

2.5. Basic Theory of Parity Non-conservation (PNC)

The dominant part of the PNC interaction can be expressed as a correction of the atomic Hamiltonian:

$$H^{PNC} = G_F Q_W \frac{1}{2\sqrt{2}} \rho(\tau) \gamma_5 \quad (45)$$

where $G_F = 2.22 \times 10^{-14}$ au gives the small size of the interaction, $\rho(\tau)$ is the nuclear density, Q_W is the weak charge and given by

$$Q_W = -N + Z(1 - 4\text{Sin}^2\theta_W) \quad (46)$$

where N and Z are the number of neutrons and electrons respectively. $\text{Sin}^2\theta_W$ is the fundamental parameter for the standard electro-weak *model*⁷³⁻⁷⁴ and γ_5 is the matrix

$$\gamma_5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (47)$$

When this matrix acts on a relativistic Dirac two component spinor it exchanges the top and the bottom components so that the resulting orbital has the opposite normal parity of the unperturbed orbital. This gives the PNC nature of the atomic weak interaction Hamiltonian.

The presence of atomic PNC weak interaction means that quantities which are normally forbidden can now occur. For example: Cs $6s \rightarrow 7s$ E1 transition is parity forbidden. In the presence of PNC interaction the orbitals become parity mixed so that there is then a non-zero matrix element or amplitude for this transition due to the opposite parity of the admixture.

$$\langle 7s^- | r | 6s^- \rangle = \langle 7s^{PNC} | r | 6s \rangle + \langle 7s | r | 6s^{PNC} \rangle \quad (48)$$

where $-$ denotes a parity mixed orbital. The $6s \rightarrow 7s$ transition amplitude, which is proportional to Q_W , can be measured experimentally. If the value of Q_W can be extracted then a value for the $\text{Sin}^2\theta_W$ can be obtained. However, in order to extract Q_W it is necessary to have a value for the PNC E1 transition matrix element. These have to be calculated separately and this is the task of atomic PNC theory. The most accurate PNC measurements have been performed on Cs and this is a single valence system the theory is relatively easy.

3 Results and discussion

Table 1 displays the Hartree-Fock (HF) and configuration-interaction (CI) J-dependent and -independent optical oscillator strengths of the inner-shell excitation $1s^2 2s^2 2p^6 3s^2 S_0^e \rightarrow 1s^2 2s^2 2p^5 3s^2 {}^2P_j^o$ transition, which leads to autoionization, of both length (f_L) and velocity (f_V) forms, in $F\epsilon^{15+}$ ion of the sodium isoelectronic sequence. It is clear from the Table that there is disagreement between the HF (f_L) and (f_V) which suggests that the correlation must be included. The CI (f_L) and (f_V) is in better agreement but the discrepancy remains which indicates the importance of the relativity. The relativity has been included in the calculation via Breit-Pauli Hamil-

4. Conclusions and future directions

tonian. The Table exhibits the J-dependent oscillator strengths and better agreement has been achieved.

Tables 2-4 show the HF and CI optical oscillator strengths of the inner-shell excitation $1s^2 2s^2 2p^6 3s^2 3p^6 3d \ ^2D^e \rightarrow 1s^2 2s^2 2p^6 3s^2 3p^5 3d^2 \ ^2P^o$, $\ ^2D^o$ and $\ ^2F^o$ transitions, which leads to autoionization, in Sc^{2+} , Ti^{3+} and V^{4+} ions of the potassium isoelectronic sequence. It is clear from Tables 2-4 that the HF (f_L) and (f_V) disagree with each other by about a factor of two. This disagreement indicates that the HF description is not adequate. It is indispensable to incorporate the correlation. The CI (f_L) and (f_V) has good agreement which demonstrates the importance of the correlation. Table 5 gives the resonance excitation energy in Li-like U^{89+} ion. The Table displays the effects of relativity, correlation, and quantum electrodynamic. The agreement between the experiment and theory is good. However, the discrepancy exists which suggests to include other physical effects, e.g., finite nuclear size (FNS), parity nonconservation (PNC). Table 6 presents the self energy in Li-like U^{89+} ion showing the effect of the nuclear size.

Blundell *et al*⁸⁰ have extensively investigated and reviewed the PNC effects (see references therein). Table 7 presents the PNC amplitude in Cs. Several calculations have been carried out. Overall, there is reasonably good agreement between the theoretical predictions and experimental observations. Table 8 gives the fundamental parameter in the standard model $Sin^2\theta_W$. The atomic physics gives good value of the $Sin^2\theta_W$ compare to the world average value which indicates that the atomic physics is capable of providing information about the weak interaction. Table 9 gives the ionization energy of Cs with the correction of PNC. It demonstrates that the PNC plays an important role in order to obtain the accurate results.

The high-precision investigation of the effects of correlation, relativity, QED, FNS and PNC by experiments provides very sensitive test of the theoretical methods. Such stringent tests are especially important as the general problem of QED and PNC theories is extremely difficult and has not been solved completely until now. Only correlation and relativity have been treated on an equal footing in the MCDF and RMBPT. The MCDF and RMBPT results are in excellent agreement with experiments which have not included the QED and PNC effects. Most experiments do not isolate these physical effects. No experiment has separated all effects. More precise experimental investigation would be desirable. Most of the theories, for examples, MCDF and RMBPT, include correlation and relativity effects simultaneously in a unified manner. However, these theories do not explain the Lamb shift which suggest to develop new theoretical methods. Several theoretical techniques are available in the literature for the calculations of QED, FNS and PNC effects independently. There is disagreement between high precision experiment and high precision theory. It is probably because that no theoretical method incorporates all effects simultaneously on an equal footing. At present, we do not have a comprehensive and practical theory that accounts all these physical effects simultaneously.

A hybrid theory, which combines the effectiveness of the MCDF method in dealing with the most obvious addition of more subtle correlation through the MBPT, provides our best hope for a unified theory that accounts for all effects simultaneously and systematically. Another direction which can exploit the close relation between the RMBPT and QED and the productive cross fertilization of these two may be capable of yielding excellent results of accuracy well below 1% level.

In short, our knowledge of high-precision electronic structure of atoms

and ions, particularly for heavy atoms and ions, is by no means complete. Comprehensive and painstaking work needs to be done and the field will continue to grow, develop and flourish. The future holds many challenges for both experiment and theory.

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Table 1.

J-independent and -dependent oscillator strengths of
 $1s^2 2s^2 2p^6 3s \ ^2S^o_J \rightarrow 1s^2 2s^2 2p^5 3s^2 \ ^2P^o_J$
in the sodium isoelectronic sequence

function	present results		other results		present results			
	f_L	f_V	f_L	f_V	$2J+1$	$2J'+1$	f_L	f_V
HF	0.064	0.060			2	2	0.022	0.019
					2	4	0.043	0.040
Cl	0.084	0.087	0.087	0.084	2	2	0.031	0.028
					2	4	0.059	0.056

Table 2.

Optical oscillator strengths of $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 D^e$
 $\rightarrow 1s^2 2s^2 2p^6 3s^2 3p^5 3d^2 {}^2 P^o$
 in the potassium isoelectronic sequence

function	Sc^{2+}		Ti^{3+}		V^{4+}	
	f_L	f_V	f_L	f_V	f_L	f_V
HF	1.18	0.63	1.12	0.59	1.03	0.54
CI	0.71	0.78	0.65	0.72	0.78	0.86

Table 3.

Optical oscillator strengths of $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 D^e$
 $\rightarrow 1s^2 2s^2 2p^6 3s^2 3p^5 3d^2 {}^2 D^o$
 in the potassium isoelectronic sequence

function	Sc^{2+}		Ti^{3+}		V^{4+}	
	f_L	f_V	f_L	f_V	f_L	f_V
HF	2.46	1.24	2.31	1.15	2.13	1.06
CI	1.40	1.16	0.56	0.44	1.82	1.55

Table 4.

Optical oscillator strengths of $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 D^e$
 $\rightarrow 1s^2 2s^2 2p^6 3s^2 3p^5 3d^2 {}^2 F^o$
 in the potassium isoelectronic sequence

function	Sc^{2+}		Ti^{3+}		V^{4+}	
	f_L	f_V	f_L	f_V	f_L	f_V
HF	1.80	1.14	1.69	1.06	1.56	0.98
CI	0.64	0.64	1.21	1.16	0.46	0.44

Table 5.

Resonance excitation $1s^2 2s^2 S_{1/2} \rightarrow 1s^2 2p^2 P_{1/2}$
 transition energy (in eV) of Li-like
 U^{89+} ion

Dirac-Fock, without Breit	286.54
Breit interaction	36.44
Correlation (RMBPT-DF)	-0.73
Hydrogenic self energy	-43.96
Self energy screening	2.38
Total screened QED corrections	-41.57
Total DF + RMBPT	280.68
Experiment	280.59 + 0.10

Table 6.

Self energy (in eV) of the $2 S_{1/2}$ and $2 P_{1/2}$ states in Li-like
 U^{89+} ion

Physical effects	$2 S_{1/2}$	$2 S_{1/2}$	$2 P_{1/2}$	$2 P_{1/2}$
Hydrogenic, point nucleus	66.38(7) ^a	66.295 ^b	9.70(7) ^a	9.625 ^b
Effect of nuclear size	-0.87(3) ^a	-0.90(6) ^c	-0.07(2) ^a	-0.10(5) ^c
Electronic screening, direct	-2.77(3) ^a	-2.75(2) ^c	-0.99(3) ^a	-0.97(2) ^c
Electronic screening, exchange	0.21(5) ^a		0.04(4) ^a	
Total self energy	62.95(8)		8.68(8)	

a: Persson, Lindgren and Salomonson⁶²

b: Mohr⁶³

c: Blundell⁵⁹

Table 7.

$Cs \ 6s \rightarrow 7s$ PNC E_1 transition amplitude
 $(\times 10^{-11} i e a_0 (-Q_W/N))$

Dzuba et al	0.91 (1 \pm 0.01)
Hartley and Sandars	0.904 (1 \pm 0.02)
Hartley et al	0.933 (1 \pm 0.04)
Johnson et al	0.951 (1 \pm 0.05)
Bouchiat and Piketty	0.935 (1 \pm 0.02 \pm 0.03)

Table 8.

Fundamental parameter in the standard model $\text{Sin}^2\theta_W$

Atomic physics	$0.226 \pm 0.007(\text{experiment}) \pm 0.004(\text{theory})$
World average	$0.2264 \pm 0.0054(\text{experiment})$

Table 9.

Ionization energy (in atomic unit) of Cs

State	ϵ	$\delta\epsilon$	Sum	Experiment
6 $S_{1/2}$	0.12737	0.01521	0.14257	0.14310
6 $P_{1/2}$	0.08562	0.00636	0.09198	0.09217
6 $P_{3/2}$	0.08379	0.00572	0.08951	0.08964

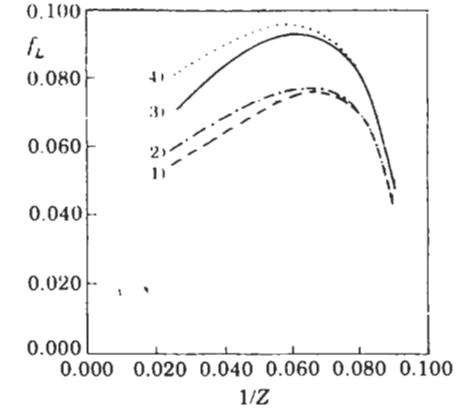


Figure 1. Theoretical oscillator strengths f_i as a function of $1/Z$ for the excitation $1s^2 2s^2 2p^6 3s^2 S_0^+ \rightarrow 1s^2 2s^2 2p^5 3s^2 P_0^+$ in the sodium isoelectronic sequence.

Curve 1, Hartree-Fock (HF);

Curve 2, HF with relativistic effect;

Curve 3, Configuration interaction (CI);

Curve 4, CI with relativistic effect;

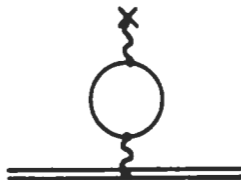


Fig. 2. Feynman diagram for the lowest-order vacuum-polarization correction for a bound electron.

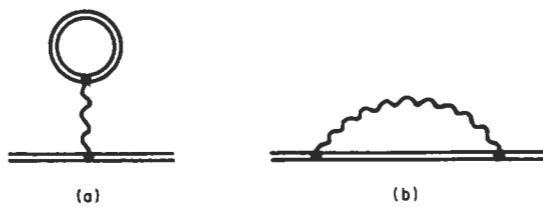


Fig. 3. Lowest-order (a) vacuum-polarization and (b) self-energy corrections to bound-electron energy levels.