REVIEW / SYNTHÈSE

Atomic calculations for tests of fundamental physics[1]

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Abstract: An overview of applications of atomic calculations for atomic physics tests of fundamental physics is presented. The current status of atomic parity violation studies is discussed in detail. The progress on the development of a novel method for precision calculation of properties of atomic systems with a few valence electrons is reported. This method combines the all-order approach currently used for monovalent atoms with the configuration interaction approach that is applicable for many-electron systems. Development of this method is aimed at significant improvement in the theoretical accuracy of the parity nonconserving amplitude calculations in systems with more than one valence electron. Tests of fundamental symmetries and other applications not only require precise calculations of the atomic properties but also evaluation of the accuracy of the results. Possible approaches to evaluating the uncertainties of the theoretical values and an example of such an evaluation are considered.

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Résumé : Nous proposons une vue d'ensemble des applications de calculs atomiques comme tests de physique fondamentale. Nous discutons en détail l'état actuel des études de violation de parité en physique atomique. Nous présentons les progrès faits dans le développement d'une nouvelle méthode pour calculer avec précision les propriétés de systèmes atomiques comptant quelques électrons de valence. Cette approche combine l'approche à tous les ordres, couramment utilisée pour les atomes monovalents, avec l'approche d'interaction de configuration qui est applicable aux systèmes à plusieurs électrons. Le développement de cette méthode vise à améliorer de façon significative la précision théorique des calculs d'amplitude de non conservation de parité dans les atomes à plus d'un électron de valence. Les tests de symétries fondamentales et d'autres applications non seulement exigent un calcul précis des propriétés atomiques, mais aussi une évaluation de la précision des résultats. Nous passons en revue les approches possibles pour évaluer théoriquement les incertitudes et présentons un exemple de calcul.

[Traduit par la Rédaction]

1. Introduction

Recent advances in experimental atomic physics, remarkable increases in computational power, and the development of the high-precision methodologies to study atomic physics quantities led not only to our better understanding of the atomic properties but also to remarkable opportunities for applications in many areas of science and technology. One such areas is the study of fundamental symmetries with atomic systems. The goals of high-precision atomic parity violation studies are to search for new physics beyond the SM (SM) of the electroweak interaction by accurate determination of the weak charge Q_W and to probe parity violation in the nucleus by evaluation of the nuclear anapole moment. Atomic parity nonconservation (PNC) measurements have been completed in Cs (0.35% accuracy [1]), Tl (1.7% [2, 3]), Bi (2% [4]), Pb (1.2% [5, 6]), as well as Sm [7] and Dy [8].

Interpretation of the cesium PNC experiment [1] requires a theoretical calculation of the parity-violating amplitude in terms of the weak charge Q_W. The most recent calculation of the PNC amplitude and consequent analysis of a Cs experiment [9] provided the most accurate low-energy test of the electroweak sector of the the SM to date. The result of this study agrees with the prediction of the SM and places constraints on a variety of new physics scenarios beyond the SM. The lower limit on the masses of extra Z bosons, predicted by the models of grand unification and string theories, was increased [9]. Combined with the results of high-energy collider experiments, the Cs PNC study [1, 9] confirmed the energy dependence (or "running") of the electroweak force

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over an energy range spanning four orders of magnitude (from ~10 MeV to ~100 GeV).

The study of PNC in cesium also led to a first measurement of the nuclear anapole moment [1] and allowed to place constraints on PNC meson coupling constants [10, 11]. These constraints were found to be in disagreement with the ones obtained from nuclear parity violating experiments. Recently, a high-precision relativistic all-order calculation of the spin-dependent PNC amplitude in Cs [12] was carried out in an attempt to understand this discrepancy. The new result [12] was found to be consistent with the older atomic physics value of the anapole coupling constant. Therefore, the disagreement between atomic and nuclear physics PNC studies remains unexplained.

More PNC experiments in other atomic systems, such as Yb [13], Fr [14–16], and Ra^+ [17], are currently in progress. In 2010, atomic parity violation was observed in the $6s^2\ ^1S_0$–$5d6s\ ^3D_1$ 408 nm forbidden transition of ytterbium [13]. The parity-violating amplitude was found to be two orders of magnitude larger than in cesium, and constitutes the largest atomic parity-violating amplitude yet observed. This experiment, carried out by D. Budker's group at the University of California, Berkeley, opened the way to future measurements of neutron distributions and anapole moments by comparing parity-violating amplitudes for various isotopes and hyperfine components of the transition.

In the case of Pb, Bi, and Tl experiments, no theoretical calculations of comparable accuracy exist to allow the full analysis of those measurements to test the SM. Development of a new theoretical approach that combines configuration interaction (CI) with coupled-cluster method [18] is aimed at a significant improvement of the theoretical accuracy.

An intrinsic electric dipole moment (EDM) can exist only if parity (P) and time reversal (T) invariance are violated [19]. The intrinsic EDMs predicted by the SM are much too small to be detected, but various extensions to the SM predict observable values. While CP violation is observed in particle physics, much stronger CP-violating mechanisms may be required to explain the matter–antimatter asymmetry of the universe. Experimental searches for EDMs provide constraints on such models. In heavy paramagnetic atoms, an electron EDM results in an atomic EDM enhanced by a factor $R = d_{\rm atom}/d_{\rm e}$ (see ref. 20 and refs. cited therein). The atomic calculations of the enhancement factors R [21] are needed for the interpretation of the EDM experiments and as a guide for a future experimental effort in the search for the EDM.

Another test of fundamental physics where the atomic physics calculations are important is the search for the variation of the fundamental constants, such as the fine-structure constant α. The astrophysical approach to such studies (involving study of absorption lines in the spectra of distant quasars) requires the calculations of the isotope shifts in many systems, since possible changes in isotopic abundances with time may mimic the variance in the value of the fine-structure constant [22]. The laboratory searches for the variation of the fundamental constants are based on comparing the frequencies of two ultra-precise atomic clocks over time [23]. Atomic calculations are needed to evaluate some uncertainties of the current atomic clocks (such as blackbody radiation shifts [24]) for the improvement of their precision, and to search for new opportunities to develop more precise frequency standards. The development of more accurate atomic clocks resulted in numerous technological applications and new opportunities for the tests of fundamental science. New generations of the atomic clocks, based on optical rather than microwave frequency standards, will increase the accuracy and stability of atomic clocks by orders of magnitude. More precise frequency standards will lead to more sensitive quantum-based standards for applications such as inertial navigation, magnetometry, gravity gradiometry, measurements of the fundamental constants, and testing of physics postulates.

2. Parity violation

The PNC effects in atoms lead to a nonzero amplitudes for atomic transitions that are otherwise forbidden by the parity selection rule, such as the 6s–7s transition in cesium. PNC effects in atoms are caused by the exchange of a virtual Z_0 boson between an electron of the atom and a quark in the nucleus, or between two atomic electrons. The second effect is extremely small, contributing only 0.03% to the PNC amplitude in Cs [25]. The dominant PNC interaction between an atomic electron and the nucleus is described by a Hamiltonian, $H^{(1)} = A_{\rm e}V_{\rm N}$, which is the product of the axial-vector electron current $A_{\rm e}$ and the vector nucleon current $V_{\rm N}$. Another contribution comes from the product of the vector electron current $V_{\rm e}$ and the axial-vector nucleon current $A_{\rm N}$, $H^{(2)} = V_{\rm e}A_{\rm N}$. Another PNC interaction that depends on the spin of the nucleus arises from the electromagnetic coupling of atomic electrons to the nuclear anapole moment, which is a parity-violating nuclear toroidal magnetic moment described in [26].

The Boulder experiment [1] resulted in the measurement of the quantities $R = {\rm Im}(E_{\rm PNC})/\beta$ for the $6s_{F=4}$–$7s_{F=3}$ and $6s_{F=3}$–$7s_{F=4}$ transitions in ^{133}Cs, where F is the total angular momentum ($I = 7/2$ for ^{133}Cs nucleus) and β is a vector transition polarizability [27]. The resulting values,

$$R_{4-3} = -1.6349(80)\ {\rm mV/cm}$$

and

$$R_{3-4} = -1.5576(77)\ {\rm mV/cm}$$

allow us to infer data for two different types of PNC effects in atoms. The *average* of R_{4-3} and R_{3-4} gives a PNC amplitude that does not depend on the nuclear spin (divided by β). The accuracy of the resulting value is very high, 0.35%. This result is combined with the theoretical $E_{\rm PNC}/Q_{\rm W}$ and either an experimental or theoretical value of β to determine the weak charge and compare it with the value predicted by the SM of the electroweak integrations [9]. In calculations, $Q_{\rm W}$ is treated as a parameter. The *difference* of R_{4-3} and R_{3-4} gives the spin-dependent PNC amplitude, divided by β. This result is combined with theoretical value of the spin-dependent PNC amplitude to probe weak hadronic integrations. The dominant contribution to the spin-dependent PNC comes from the nuclear anapole moment. We note that the difference of R_{4-3} and R_{3-4} was measured with only 14% accuracy.

We consider nuclear spin-independent and spin-dependent effects separately. While the methods of the calculation the PNC amplitudes are the same, the Hamiltonians of the two interactions are entirely different.

2.1 Spin-independent PNC and weak charge

The time-like component of the $A_e V_N$ interaction leads to the dominant PNC effect, caused by the exchange of a virtual Z_0 boson between an electron of the atom and a quark in the nucleus. It can be reduced to an effective Hamiltonian in the electron sector [28],

$$H_{\rm PNC} = \frac{G_{\rm F}}{2\sqrt{2}} Q_{\rm W} \gamma_5 \rho(r) \tag{1}$$

where $G_{\rm F}$ is the universal Fermi coupling constant, and γ_5 is the Dirac matrix associated with pseudoscalars. The quantity $Q_{\rm W}$ is the weak charge, defined by,

$$Q_{\rm W} = -N + Z(1 - 4\sin^2\theta) \tag{2}$$

where N is the neutron number, Z is the proton number, and θ is the Weinberg angle. Since $\sin^2\theta \approx 1/4$, it follows that $Q_{\rm W} \approx -N$. The quantity $\rho(r)$ is a nuclear density function, which is approximately the neutron density. The issue of the nuclear density functions was discussed in detail in [29].

There are two approaches to calculating the PNC amplitude, (*i*) via the direct solution of the perturbed Dirac equation and subsequent evaluation of the forbidden dipole matrix element and (*ii*) using the sum-over-states method. There are advantages and disadvantages to both methods.

In lowest order many-body perturbation theory, which includes the perturbation of the DHF potential induced by the weak interaction $\widetilde{V}_{\rm HF}$, one first solves the perturbed Dirac equation [28],

$$(h_{\rm D} + V_{\rm nuc} + \widetilde{V}_{\rm HF} + H_{\rm PNC})\widetilde{\psi} = \epsilon\widetilde{\psi} \tag{3}$$

Then, one evaluates the forbidden dipole matrix element z_{vw} between states v and w as,

$$E_{\rm PNC} = \langle\psi_w|D|\widetilde{\psi}_v\rangle + \langle\widetilde{\psi}_w|D|\psi_v\rangle \tag{4}$$

where D is the electric-dipole operator. The system of perturbed core and valence equations is solved self-consistently, leading to the first-order PNC amplitude in Cs,

$$E_{\rm PNC} = 0.927\,\frac{i|e|a_0 Q_{\rm W}}{-N} \times 10^{-11}$$

where a_0 is the Bohr radius. Starting from the weak amplitude in lowest order, one evaluates the corrections in second- and third-order by weakly perturbing all orbitals appearing in expressions for the second- and third-order dipole matrix elements. Certain classes of the dominant all-order corrections are incorporated using the correlation potential method [30]. The advantages of the correlation potential method are discussed, for example, in [31].

In the direct sum-over-states approach [28], one considers the sum,

$$E_{\rm PNC} = \sum_n \frac{\langle\Psi_w|D|\Psi_n\rangle\langle\Psi_n|H_{\rm PNC}|\Psi_v\rangle}{E_v - E_n} + \sum_n \frac{\langle\Psi_w|H_{\rm PNC}|\Psi_n\rangle\langle\Psi_n|D|\Psi_v\rangle}{E_w - E_n} \tag{5}$$

For the $6s_{1/2}$–$7s_{1/2}$ transition in Cs, the intermediate states range over all $np_{1/2}$ states. The dominant terms, n = 6, 7, 8, 9, are evaluated, for example, using the all-order (linearized coupled-cluster) method (see [32] for a review of the formulation and applications of the all-order method). The theoretical error in these calculations is estimated by replacing ab initio theoretical data in the sums by precisely known experimental data or modified theory values, which include semi-empirical estimates of the omitted correlation effects, and noting the changes in the partial sum [28]. Contributions from terms with n = 2 to 5 and n = 10 to ∞ are evaluated in the weak RPA approximation in a finite basis set. The advantage of this approach is the explicit, very accurate evaluation of the dominant terms with low n and the ability to replace certain matrix elements by high-precision experimental values in a transparent way. The main disadvantage of the this approach is the need to evaluate the tail with $n > 9$. In the direct solution method, the tail terms are automatically included. While both approaches include different terms, the final results are remarkably close [9, 25, 28, 31, 33, 34].

Earlier calculations of the PNC amplitude in Cs carried out in 1984–1987 [35–38] have been performed using the Dirac–Hartree-Fock (DHF) method, random-phase approximation (RPA), or semi-empirical potentials. Dzuba et al. [39] included second-order many-body perturbation theory (MBPT) corrections beyond RPA. Third-order MBPT calculation of the PNC amplitude has been reported in [40]. The first calculation the PNC amplitude that included higher order correlation corrections was carried out by Dzuba et al. [33] and was reported to be accurate to 1%. Three dominant subsequences of diagrams in the correlation correction to amplitude were summed to all orders: screening of the electron–electron interaction, particle–hole interaction, and the iterations of the self-energy. The result of [31] was obtained using the same correlation potential method, but additional terms were included. Extensive study of the accuracy of the final result was performed, and 0.5% uncertainty was reported.

Another all-order calculation was carried out by Blundell et al. [25] in 1990 using a different (relativistic linearized coupled-cluster) approach. Extensive study of the accuracy of this approach (1%) was carried out in [28], and some additional corrections were added. Another high-precision calculation was carried out in [34]. All these high-precision results were found to be in excellent agreement with each other.

The most accurate evaluation of the spin-independent amplitude to date was carried out in [9] using the CCSDVT method (coupled-cluster method, including single, double, and valence triple excitations). Their result,

$$E_{\rm PNC} = 0.8906\,\frac{i|e|a_0 Q_{\rm W}}{-N} \times 10^{-11}$$

is accurate to 0.3%. This calculations incorporated other non-Coulomb corrections to the PNC amplitude, including Breit (0.6%) [41, 42], QED (0.3%) [43], neutron skin [29] (0.2%), and e–e weak interaction corrections (0.03%) [25]. Combining the final theoretical value of $E_{\rm PNC}$ with the value of vector transition polarizability, $\beta = -26.957(51)\,a_0^3$ [31], and experimental measurements from [1], yielded the value of the weak charge [9],

$$Q_{\rm W}(^{133}{\rm Cs}) = -73.16(29)_{\rm expt}(20)_{\rm theor}$$

that is in agreement with the value predicted by the SM [44],

$$Q_W^{SM} = -73.16(3)$$

Combined with the results of high-energy collider experiments, the Cs PNC study [1, 9] confirmed the energy dependence (or "running") of the electroweak force. The close agreement of Cs PNC study with the SM prediction places constraints on a variety of new physics scenarios beyond the SM.

We note that the determination of the parity-conserving quantities, such as transition matrix elements, lifetimes, polarizabilities, and hyperfine constants, is essential for PNC studies. The electric-dipole matrix elements contribute directly to the PNC amplitude calculated using the sum-over-states approach and to the evaluation of the vector transition polarizability β. Evaluation of the other quantities is needed in part to demonstrate accuracy of the theoretical approaches. We stress that an evaluation of the theoretical uncertainty is required for the interpretation of the PNC study, in terms of the comparison with the SM. We discuss the evaluation of the theoretical uncertainty in Sect. 3.

A program to measure PNC in Fr has been underway for the past decade [14, 15]. An experiment to measure the nuclear spin-dependent PNC amplitude between ground-state hyperfine levels in Fr isotopes was proposed in [45]. The (currently approved) plans for Fr on-line laser trapping at the ISAC radioactive beam facility at TRIUMF, for a measurement of the nuclear anapole moment, are described in [14]. Production and trapping of Fr ions has also been reported in [16]. Correlation potential and relativistic all-order (linearized coupled-cluster) calculations of the E_{PNC} for the $7s_{1/2}$–$8s_{1/2}$ transition in francium were carried out in [46, 47], respectively. At the present time, there is a 3% discrepancy between the correlation potential and coupled-cluster values. Both calculations quote 1% accuracy. An investigation of the sources of the discrepancy in [47] noted a 0.6% difference owing to the use of different nuclear parameters in the two calculations and a 1% difference from the Breit interaction, which was omitted in the calculation of [46].

A project to measure PNC in a single trapped radium ion recently started at the Accelerator Institute (KVI) of the University of Groningen [17]. PNC amplitude in Ra^+ has been evaluated in [48–50]. Parity-nonconserving s–d amplitudes in Cs, Fr, Ba^+, and Ra^+ have been calculated in [49], using a hybrid mixed-states sum-over-states approach.

PNC studies have been carried out for the $6p_{1/2}$–$6p_{3/2}$ transition in ^{205}Tl in Oxford [2] and Seattle [3]; for the $6\ ^3P_0$–$6\ ^3P_1$ transition in ^{208}Pb in Seattle [5] and Oxford [6]; and for the $^4S_{3/2}$–$^2D_{3/2}$ transition in ^{209}Bi in Oxford [4]. Re-measurement of the $E2/M1$ ratio for the $6p_{1/2}$–$6p_{3/2}$ transition in Tl [51] helped reconcile differences between the Oxford and Seattle measurements for that atom. The most recent calculation of the PNC amplitude in Tl [34] was estimated to be accurate to about 3%.

The $(6s2)^1S_0$–$(6s5d)^3D_1$ PNC transition in atomic Yb is about 100 times larger than the 6s–7s transition in cesium [52], being enhanced by mixing of the final state with the nearby $(6s6p)^1P_1$ state. A recent experiment [13] confirmed such a large PNC effect. Measurements of PNC in ytterbium are particularly interesting, since there are seven naturally occurring isotopes, $^{168–176}$Yb, giving the possibility of eliminating uncertainties arising from atomic structure calculations by comparing PNC amplitudes from different isotopes. The best many-body calculation of the PNC amplitude in Yb [53] gave a value accurate to about 20%. In Sect. 4, we discuss a novel approach that combines linearized coupled-cluster method used in evaluation of the Cs PNC amplitude with the CI approach. The development of this method is aimed at a significant improvement of the theoretical accuracy.

A Stark interference experiment to detect PNC mixing between two nearly degenerate levels of opposite parity, $(4f^{10}5d6s)$ [10] and $(4f^95d^26s)$ [10] in dysprosium has been carried out [8]. This experiment gave a result that differed substantially from the theoretical result obtained in a multiconfiguration Dirac–Fock (CI) calculation [54]. Optical rotation parameters for transitions between ^7F_J and $^5D_{J'}$ states in the $(4f^66s^2)$ multiplet of samarium were measured [7]. The upper state levels are nearly degenerate, with levels of opposite parity from the $(4f^66s6p)$ configuration, leading to an expected enhancement of the PNC amplitude. The weak interaction matrix elements $|H_W|$, extracted from experiment, ranged from 1 to 30 kHz, which was one to two orders of magnitude smaller than what was expected from semi-empirical calculations. Significant improvement in theoretical methodology is needed to provide reliable estimate of the PNC effects in these complicated systems.

2.2 Spin-dependent PNC and anapole moment

The spin-dependent contribution to the PNC amplitude has three distinct sources: the nuclear anapole moment, the Z-exchange interaction from nucleon axial-vector currents (A_nV_e), and the combined action of the hyperfine interaction and spin-independent Z-exchange from nucleon vector (V_nA_e) currents. The anapole moment contribution strongly dominates. The nuclear anapole moment and the Z-exchange interaction from nucleon axial-vector currents (A_nV_e) interactions can be represented by the same Hamiltonian,

$$H^{(i)} = \frac{G}{\sqrt{2}}\kappa_i \boldsymbol{\alpha}\cdot\boldsymbol{I}\rho(r) \tag{6}$$

In the equation above, subscript $i = a$, 2 refers to the anapole moment and the axial-vector contributions, respectively; G is the universal weak coupling constant, $\boldsymbol{I}$ is the nuclear spin, and $\rho(r)$ is a normalized nuclear density function. The dimensionless constant κ_a is used to characterize the anapole moment [55]. The constant $\kappa_2 = 0.0140$ was calculated in [55]. The total spin-dependent PNC contribution to the electric-dipole matrix element $\langle 7sF_F||z||6sF_I\rangle$ is given by [56],

$$\langle 7sF_F \parallel D \parallel 6sF_I\rangle_{PNC} = (\kappa_a + \kappa_2 + \kappa_{hf})\langle 7sF_F \parallel D \parallel 6sF_I\rangle^{(2,a)} \tag{7}$$

The combined hyperfine and the spin-independent Z-exchange interactions are characterized by the constant κ_{hf}. It was calculated using the random-phase approximation (RPA) to be $\kappa_{hf} = 0.0049$ in [56].

In [57], the spin-dependent PNC amplitude was evaluated using a semi-empirical method. DHF calculation was carried out in [28]. The relativistic Hartree–Fock method and Brueckner orbitals were used in [58].

The study of PNC in cesium led to a first measurement of the nuclear anapole moment and allowed to place constraints

on PNC meson coupling constants [10, 11, 55, 59]. These constraints were found to be in disagreement with the ones obtained from nuclear parity violating experiments. These determinations of the PNC meson coupling constants were based on the calculation of the main part of the spin-depended PNC amplitude from [57, 58].

The discrepancy of the nuclear and atomic PNC studies motivated further study of the spin-depended amplitude. In [12], the spin-depended $E_{\rm PNC}$ was calculated using a relativistic all-order method to about 1% precision. Combining the theoretical results for the spin-dependent PNC amplitude with the experimental value of $\Delta[{\rm Im}(E_{\rm PNC})/\beta]_{34-43} = -0.0077(11)$ mV/cm from [1], and $\beta = 27.02(8)\,a_0^3$ [27]; Safronova et al. [12] obtained the result $\kappa = \kappa_{\rm a} + \kappa_2 + \kappa_{\rm hf} = 0.107(16)$. This value is rather close to the previous value of 0.112(16) from [10]. The uncertainty in both values is the experimental one (14%).

Safronova et al. [12] reported that individual PNC matrix elements significantly change with a more complete inclusion of the correlation corrections, whereas changes in the total spin-dependent PNC amplitude are relatively small. The value of the anapole coupling constant $\kappa_{\rm a} = 0.88(12)$ calculated in [12] is only 5% lower than the value used in [10, 59]. Therefore, a more accurate evaluation of the spin-depended PNC in Cs did not resolve the discrepancies in the constraints on PNC meson coupling constants. We note that analysis of nuclear parity violation within the framework of effective field theory (EFT) is being reformulated at the present time [60].

Further experiments capable of accurate measurement of the spin-depended PNC interaction effects are needed for further understanding of the discrepancies between nuclear and atomic PNC studies.

3. Evaluation of theoretical uncertainties

We have shown above that the analysis of the PNC studies requires the evaluation of the complete (rather than numerical) theoretical uncertainties. Many other applications (for example, evaluation of the blackbody radiation shifts for atomic clock research) require such studies as well. This issue was discussed in detail in a review of the blackbody radiation shift calculations [24]. Benchmark comparisons of theory and experiment carry more value when the theoretical results are accompanied by uncertainty evaluations. Evaluations of the theoretical uncertainties are still rare and cannot be carried out in all cases and for all of the methods. Below, we discuss how some theoretical uncertainties may be evaluated. The sum-over-states approach to the calculation of the PNC amplitude discussed above is based on the evaluation of the various types of matrix elements. Therefore, it is necessary to be able to evaluate uncertainties of the individual matrix elements (for example, E1 matrix elements) to evaluate final uncertainties of the composite quantities, such as PNC amplitude. We discuss the evaluation of the uncertainties in the results obtained by the relativistic all-order method [32]. The strategies to evaluate the uncertainties of the matrix elements within the framework of this approach include the approximate evaluation of the size of the correlation correction, evaluation of the size of the higher order corrections, study of the order-by-order convergence of perturbation theory, study of the breakdown of the various all-order contributions and identification of the most important terms, and semi-empirical determination of dominant missing contributions. We illustrate these strategies using the example of the calculation of the atomic quadrupole moment of the $3d_{5/2}$ state in Ca^+ [61]. This is the most extensive evaluation of the uncertainty in a single matrix element to our knowledge. It was motivated by some controversy between other high-precision calculations and experimental measurement (see [61] for the discussion of this issue). Moreover, this property has been measured to rather high precision (1%) in [62].

The atomic quadrupole moment $\Theta(\gamma J)$ is a diagonal matrix element of the electric quadrupole (E2) operator, defined as,

$$\Theta(\gamma J) = \frac{(2J)!}{\sqrt{(2J-2)!(2J+3)!}} \langle \Psi(\gamma J) \parallel Q \parallel \Psi(\gamma J) \rangle \qquad (8)$$

Strategies to evaluate its uncertainty require evaluations of $\Theta(\gamma J)$ in as many different approximations of the increased accuracy as possible. We list the value of the quadrupole moment of the $3d_{5/2}$ state in Ca^+, calculated using the ab initio lowest order and third-order many-body perturbation theory (MBPT), single-double linearized coupled-cluster method (LCCSD), single-double linearized coupled-cluster method with partial valence triple excitations (LCCSDvT), and single-double coupled-cluster approach (CCSD) with all SD nonlinear terms included. All data are listed in atomic units.

Lowest-order 2.451
Third-order 1.610
LCCSD 1.785
LCCSDvT 1.837
CCSD 1.822

The sequence of these values gives the estimate of the contribution of the correlation corrections as well as importance of the fourth and higher order correction, nonlinear terms, and triple excitations. The final evaluation of the uncertainty required identification and elaborate semi-empirical evaluation of the missing correlation effects [28, 32]. We note that the scaling factors are different in the cases of the LCCSD, LCCSDvT, CCSD methods, since they depend on the correlation energies obtained in these approximations.

LCSSDvT 1.837
LCCSD scaled 1.849
LCSSDvT scaled 1.836
CCSD scaled 1.851
Final 1.849(13)
Expt. 1.83(1)

The spread in the resulting scaled values and the ab initio LCCSDvT values that represent the most complete ab initio result is taken as the uncertainty of the final (scaled LCCSD) result. The evaluation of the theoretical uncertainties has been discussed the detail in the recent review [63].

4. CI + all-order method

The relativistic all-order [32] and correlation potential [30] methods yielded very accurate results for the PNC amplitude and other properties of the monovalent systems, such as Cs, Ba^+, Fr, and Ra^+. However, neither of this methods can be straightforwardly extended to evaluate the PNC amplitudes in more complicated systems such as Tl or Yb. In the case

of the all-order method, the number of terms in the matrix element expression increases from twenty for the monovalent systems to hundreds for divalent systems. Moreover, the all-order method is based on the Rayleigh–Schrödinger many-body perturbation theory. Use of this approach for the two-particle systems will result in the problem of accidentally small denominators and resulting divergencies in the iteration procedures. Generally, perturbative approaches are not well-suited for the treatment of the very strong valence–valence interactions. Therefore, the CI method was combined with the second-order many body perturbation theory (MBPT) in [64] to use the advantages of both methods. The CI + MBPT approach allows one to incorporate core excitations in the CI method by constructing an effective Hamiltonian that includes certain perturbation theory terms. The CI method is then implemented with the modified H^{eff} to obtain improved energies and wave functions. This method was applied to the calculation of atomic properties of various systems in a number of works (see [65–69] and refs. cited therein). In particular, it was applied to the evaluation the PNC amplitudes in Tl [34] and Yb [53]. The main problem of this approach is the deterioration of its accuracy for heavier systems owing to incomplete inclusion of the core-valence corrections, in particular for the two-body part of the effective Hamiltonian.

Using the all-order (linearized coupled-cluster) approach to construct the effective Hamiltonian leads to much more complete inclusion of the correlation correction. In the CI + all-order approach, the effective Hamiltonian is first constructed using the second-order MBPT. Then, the most important terms are recalculated using the all-order method. Therefore, the core–core and core–valence sectors of the correlation corrections for systems with a few valence electrons are treated with the same accuracy as in the all-order approach for the monovalent systems. The CI method is used to treat valence–valence correlations. This method was first introduced in [70]. Numerous tests have been conducted to establish that numerical errors (associated with the size of the initial B-spline finite basis set, saturation of the CI space, and the selection of the second-order and all-order subsets) are below the expected accuracy of the method. Comparisons of the CI + MBPT and CI + all-order binding energies for the ground and excited states of a number of two-electron systems demonstrate that the CI + all-order energies are usually more accurate by at least a factor of three [70]. The preliminary calculations of polarizabilities in Ca and Sr indicate significantly better agreement of the CI + all-order ab initio results with recommended values from [71], in comparison with the CI + MBPT approach. At the present time, the corrections to the one-body operators, such as electric-dipole or PNC operators, are only done at the random-phase approximation level in the CI + all-order approach. In the next steps of the CI + all-order method development, the full all-order terms excluding the ones accounted for by the CI part of the calculation will be included for further improvement of its accuracy. Next, the triple excitations will be included perturbatively. At that level of the inclusion of the correlation correction, the method should be sufficiently complete to carry out the evaluation of the PNC amplitudes in Tl and Yb with significant improvement of the accuracy, in comparison with the previous best calculations.

5. Conclusion

We reviewed applications of the atomic calculations to the study of fundamental interactions, in particular parity violation. The present status of the theoretical calculations of the PNC amplitude and experimental progress in various systems was discussed. The theoretical precision in the PNC amplitude calculation in Cs has finally improved to exceed the experimental uncertainty [1], stimulating the need for further experimental progress. In the case of divalent and more complicated systems, a significant improvement in theoretical precision is needed. Progress in the development of the new high-precision method, combining the linearized coupled-cluster method with configuration integrations, was discussed. The development of this method is aimed at bridging the gap between the accuracy of the theoretical and experimental PNC studies for more complicated systems.

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