Permanent Electric Dipole Moments of Closed Shell Atoms

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by

Yashpal Singh

Under the Supervision of

Dr. Bijaya Kumar Sahoo

Associate Professor

Theoretical Physics Division

Physical Research Laboratory

Ahmedabad, India.

DEPARTMENT OF PHYSICS
MOHANLAL SUKHADIA UNIVERSITY
UDAIPUR
Year of submission: 2015

To

My Parents

and to

Arti

DECLARATION

I, **Mr. Yashpal Singh**, *S/o Mr. M. P. Singh, resident of Room No. 19 UN Hostel, Physical Research Laboratory, Navrangpura, Ahmedabad, 380009, hereby declare that the research work incorporated in the present thesis entitled,* **"Permanent Electric Dipole Moments of Closed Shell Atoms"** *is my own work and is original. This work (in part or in full) has not been submitted to any University for the award of a Degree or a Diploma. I have properly acknowledged the material collected from secondary sources wherever required. I solely own the responsibility for the originality of the entire content.*

Date:

Yashpal Singh

(Author)

CERTIFICATE

I feel great pleasure in certifying that the thesis entitled **"Permanent Electric Dipole Moments of Closed Shell Atoms"** embodies a record of the results of investigations carried out by Mr. Yashpal Singh under my guidance. He has completed the following requirements as per Ph.D regulations of the University:

(a) Course work as per the university rules.

(b) Residential requirements of the university.

(c) Regularly submitted six monthly progress reports.

(d) Presented her work in the departmental committee.

(e) Published minimum of one research papers in a referred research journal.

I am satisfied with the analysis, interpretation of results and conclusions drawn. I recommend the submission of thesis.

Date:

Dr. Bijaya Kumar Sahoo
(Thesis Supervisor)
Associate Professor, THEPH,
Physical Research Laboratory,
Ahmedabad - 380 009

Countersigned by

Head of the Department

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Physical Research Laboratory

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ABSTRACT

Violations under the discrete symmetry transformations, like parity (P), time-reversal (T) and combined charged-conjugation-parity (CP) symmetries, have already been observed in nature at the elementary particle level. However, in the composite systems like atoms, P and T-violating (P,T-odd) interactions between its constituent particles could give rise to net intrinsic electric dipole moment (EDM) of the system. Therefore, observation of a non-zero EDM in an atomic system would be a clean signature of violations of both the P- and T- symmetries. In addition, atomic EDMs can also probe CP-violation originating from leptonic, semileptonic and hadronic CP sources. Since last six decades, several attempts have been made by physicists in both the high-energy and low-energy sectors to probe such CP-odd sources.

The EDMs of closed-shell (diamagnetic) atoms ($d_{\rm A}$) arise predominantly from the P,T-odd electron-nucleus (e-N) tensor-pseudotensor (T-PT) interactions and interactions between the nuclear Schiff moment (NSM) with the atomic electrons. It is assumed that NSM originates primarily due to the distorted charge distribution inside a finite size nucleus caused by the P,T-odd interactions among the nucleons mediated by the neutral pions (π^0-mesons) and due to EDMs of the nucleons. Further, at the quantum chromodynamics (QCD) energy scale, the origin of NSM can be viewed as the P,T-odd interactions among the constituent quarks and due to the EDMs and chromo-EDMs of the quarks.

Accurate theoretical evaluations of EDMs require sophisticated many-body methods, which can treat both the electron-correlation effects and the relativistic corrections adequately. In past, several lower-order many-body methods have been employed to study these properties in the atomic systems that are under consideration by the experimentalists to measure their EDMs. Validity of these methods are not well investigated and from the theoretical prospectives, they do not appear to present reliable results. The main objective of this work is to develop more accurate all-order perturbative many-body methods in the relativistic framework so that calculations obtained using these methods can be

combined with the experimental values of the EDMs for different closed-shell atomic systems to infer fundamental quantities that can be used to test possible new physics of elementary particles. In this view, we have developed methods based on the relativistic coupled-cluster (RCC) theory considering full singles and doubles approximation with linear terms (LCCSD method) and including all non-linear terms (CCSD method). To further improve our CCSD results, we perturbatively take into account contributions from the important triple excitations due to the electron-electron repulsion (CCSD(T) method) and along with the P,T-odd interaction (CCSD_pT method). In order to compare our EDM results with the previously reported values we developed a method based on random phase approximation (RPA). In addition to that, we have also developed a third-order many-body perturbation theory (MBPT(3)) and studied trends in the behavior of electron-correlation effects going from one method to another in the evaluation of the property of interest. Before performing EDM calculations, we test the potential of our many-body methods by evaluating electric dipole polarizability (α) of various closed-shell atomic system and comparing these results with the available measurements and other calculations. Since the evaluation of d_{A} and α demands similar angular momentum and parity selection criteria, but accuracies of αs can be tested against their experimental values. This, therefore, can serve as benchmark to determine EDMs reliably. After rigorous testing of our developed many-body methods, we finally evaluate d_A due to T-PT and NSM interactions of the experimentally considered atoms like ^{129}Xe, ^{199}Hg, ^{223}Rn and ^{225}Ra. Till date, the best atomic measurement on d_{A} is obtained from ^{199}Hg as $|d_A(^{199}\text{Hg})| < 3.1 \times 10^{-29}|e|$cm (at 95% confidence level). Large discrepancies among the previously reported calculated results using a variety of many-body methods have been noticed. In this thesis, we aim to explain the reasons for observing such differences by systematically including higher-order corrections to the many-body methods. With above many-body methods in hand we rigorously demonstrate the trends in the electron-correlation effects in determining α and d_{A}. We find that non-RPA contributions (pair-correlation effects) which are already there in CCSD are very crucial in achieving better accuracies in these

results. The contributions from important triple excitations to α and d_{A} were also found to be very significant (sometime 3%). Finally, we present the recommended EDM results from a method that takes into account more physical effects. On combining our recommended EDM results with the measured value of ^{199}Hg, we obtain limits on the T-PT coupling constant as $C_T < 2.09 \times 10^{-9}$ and on the NSM as $S < 1.45 \times 10^{-12}|e|\mathrm{fm}^3$. Using these values together with the latest nuclear structure and QCD calculations, we get limits for the strong CP parameter as $|\bar{\theta}| < 1.1 \times 10^{-9}$ and for the combined up- and down- quark chromo-EDMs as $|\tilde{d}_u - \tilde{d}_d| < 2.8 \times 10^{-26}|e|\mathrm{cm}$. Experiments to measure EDMs in ^{129}Xe and ^{225}Ra are actively underway aiming to improve the precision of the measurements so that the new results can surpass the upper limit set by the Hg experiment. In fact, a research group at Argonne National Laboratory has recently reported their first EDM measurement on ^{225}Ra atom. Though, their obtained limit is not competitive with Hg at present but from the theoretical and experimental point of view, ^{225}Ra has the potential to enhance this effects significantly.

In brief, a comprehensive study of closed-shell atomic EDMs is presented in this thesis with a focus on various relativistic many-body methods including the RCC theory. We highlight the importance of non-RPA contributions in determining accurate results of α and d_{A} in various closed-shell atomic systems. Our obtained limits on various P,T-odd couplings from ^{199}Hg could constraint various extensions of the standard model (SM) of particle physics. These constraints can further useful for probing new physics beyond-SM.

Keywords: Electric Dipole Moment, CPT Theorem, Dipole Polarizability, Parity, Charge-Conjugation, Time-Reversal, CP-Violation, Tensor-Pseudotensor Interaction, Nuclear Schiff Moment, Many-Body Perturbation Theory, Random Phase Approximation, Relativistic Coupled-Cluster Theory, Standard Model.

LIST OF PUBLICATIONS

Publications contributing to this thesis :

1. *Correlation trends in the ground-state static electric dipole polarizabilities of closed-shell atoms and ions*,
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3. *Correlation trends in the polarizabilities of atoms and ions in the boron, carbon, and zinc homologous sequences of elements*,
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4. *Relativistic Many-Body Analysis of the Electric Dipole Moment of* ^{223}Rn,
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5. *Rigorous limits on the hadronic and semi-leptonic CP-violating coupling constants from the electric dipole moment of* ^{199}Hg,
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Other publications :

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4. *Implementation and application of the relativistic equation-of-motion coupled-cluster method for the excited states of closed-shell atomic systems*, D. K. Nandy, **Yashpal Singh** and B. K. Sahoo, Phys. Rev. A **89**, 062509 (2014).

List of Abbreviations

A	Atomic Mass
C	Charge Conjugation
P	Parity
T	Time Reversal
T-PT	Tensor-Pseudotensor
HF	Hartree-Fock
DF	Dirac-Fock
DC	Dirac-Coulomb
DK	Douglas-Kroll
GTO	Gaussian Type Orbitals
EDM	Electric Dipole Moment
PNC	Parity Non-Conservation
QCD	Quantum Chromodynamics
QED	Quantum Electrodynamics
DM	Dark Matter
S	Schiff Moment
SM	Standard Model
SUSY	Super Symmetry
BSM	Beyond Standard Model
SCF	Self Consistent Field
MBPT	Many-Body Perturbation Theory
MDM	Magnetic Dipole Moment
CC	Coupled-Cluster
RPA	Random Phase Approximation
NCC	Normal Coupled-Cluster
NSM	Nuclear Schiff Moment
ECC	Extended Coupled-Cluster
CI	Configuration Interaction
CPHF	Coupled Perturbed Hartree Fock
TDHF	Time Dependent Hartree-Fock
CCSD	Coupled-Cluster Singles Doubles
LCCSD	Linearized CCSD
CCSD(T)	CCSD with Partial Triples
SE	Self Energy
VP	Vacuum Polarization
RCC	Relativistic CC
WK	WichmannKroll
Z	Atomic Number

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