## Permanent Electric Dipole Moments of Closed Shell Atoms

#### A THESIS

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by

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Ahmedabad, India.

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

# To

# My Parents

and to

Arti

deskpok

## 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.

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# 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.

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(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.

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Countersigned by Head of the Department

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### ABSTRACT

Violations under the discrete symmetry transformations, like parity (P), timereversal (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 ( $d_A$ ) 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 ( $\pi^0$ -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 ( $\alpha$ ) of various closed-shell atomic system and comparing these results with the available measurements and other calculations. Since the evaluation of  $d_{\rm A}$  and  $\alpha$  demands similar angular momentum and parity selection criteria, but accuracies of  $\alpha$ s 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 <sup>129</sup>Xe, <sup>199</sup>Hg, <sup>223</sup>Rn and  $^{225}$ Ra. Till date, the best atomic measurement on  $d_A$  is obtained from  $^{199}$ Hg as  $|d_A(^{199}\text{Hg})| < 3.1 \times 10^{-29} |e| \text{cm}$  (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  $\alpha$ and  $d_{\rm A}$ . 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  $\alpha$  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 <sup>199</sup>Hg, we obtain limits on the T-PT coupling constant as  $C_T < 2.09 \times 10^{-9}$ and on the NSM as  $S < 1.45 \times 10^{-12} |e| \text{fm}^3$ . 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  $|\tilde{d}_u - \tilde{d}_d| < 2.8 \times 10^{-26} |e|$ 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 <sup>225</sup>Ra atom. Though, their obtained limit is not competitive with Hg at present but from the theoretical and experimental point of view, <sup>225</sup>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  $\alpha$  and  $d_A$  in various closed-shell atomic systems. Our obtained limits on various P,T-odd couplings from <sup>199</sup>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 :

- Correlation trends in the ground-state static electric dipole polarizabilities of closed-shell atoms and ions,
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- Ab initio determination of the P- and T-violating coupling constants in atomic Xe by the relativistic-coupled-cluster method,
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- Correlation trends in the polarizabilities of atoms and ions in the boron, carbon, and zinc homologous sequences of elements,
   Yashpal Singh and B. K. Sahoo, Phys. Rev. A 90, 022511 (2014).
- 4. Relativistic Many-Body Analysis of the Electric Dipole Moment of <sup>223</sup>Rn,
  B. K. Sahoo, Yashpal Singh and B. P. Das, Phys. Rev. A 90, 050501 (2014).
- 5. Rigorous limits on the hadronic and semi-leptonic CP-violating coupling constants from the electric dipole moment of <sup>199</sup>Hg,
  Yashpal Singh and B. K. Sahoo, Phys. Rev. A 91, 030501(R) (2015).
- 6. Electric dipole moment of <sup>225</sup>Ra due to P- and T-violating weak interactions,

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#### Other publications :

1. Sc III Spectral Properties of Astrophysical Interest,

D. K. Nandy, Yashpal Singh, B. K. Sahoo and C. Li, J. Phys. B: At.
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- 4. Implementation and application of the relativistic equation-of-motion coupledcluster 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).

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# List of Abbreviations

		1. 1. 3.5
	A	Atomic Mass
	C	Charge Conjugation
	Р	Parity
	Т	Time Reversal
	Т-РТ	Tensor-Pseudotensor
	$_{ m HF}$	Hartree-Fock
	$\mathrm{DF}$	Dirac-Fock
	DC	Dirac-Coulomb
	DK	Douglas-Kroll
	GTO	Gaussian Type Orbitals
	EDM	Electric Dipole Moment
	PNC	Parity Non-Conservation
	$\rm QCD$	Quantum Chromodynamics
	QED	Quantum Electrodynamics
	DM	Dark Matter
	$\mathbf{S}$	Schiff Moment
	$\mathbf{SM}$	Standard Model
	SUSY	Super Symmetry
	BSM	Beyond Standard Model
	$\mathbf{SCF}$	Self Consistent Field
	MBPT	Many-Body Perturbation Theory
	MDM	Magnetic Dipole Moment
	$\mathbf{C}\mathbf{C}$	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
$\sim$	SE	Self Energy
<b>U</b>	VP	Vacuum Polarization
	RCC	Relativistic CC
	WK	WichmannKroll
	Z	Atomic Number

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