Studies Towards the Possible Temporal Variation of the Fine Structure Constant

A thesis submitted in partial fulfillment of
the requirements for the degree of

Doctor of Philosophy

by

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DISCIPLINE OF PHYSICS

INDIAN INSTITUTE OF TECHNOLOGY GANDHINAGAR

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to

my family

Declaration

I declare that this written submission represents my ideas in my own words and where others' ideas or words have been included, I have adequately cited and referenced the original sources. I also declare that I have adhered to all principles of academic honesty and integrity and have not misrepresented or fabricated or falsified any idea/data/fact/source in my submission. I understand that any violation of the above can cause disciplinary action by the Institute and can also evoke penal action from the sources which have thus not been properly cited or from whom proper permission has not been taken when needed.

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CERTIFICATE

It is certified that the work contained in the thesis titled "**Studies Towards the Possible Temporal Variation of the Fine Structure Constant**" by DILLIP KUMAR NANDY (11330002), has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

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Abstract

In the standard model (SM) of particle physics it is a well-known fact that coupling constants of different fundamental interactions run with energy. The variations of these coupling constants under different local energy regimes have already been verified experimentally. But in the current scenario there is no law or symmetry principle, other than a presumption for the sake of simplicity, that restrains the physical constants of nature from varying in space and time. Hence, it is necessary to verify this assumption experimentally.

Investigations of temporal variation of fundamental constants have been gaining the ground steadily in both the theoretical and experimental physics for the last two decades [J. P. Uzan, Rev. Mod. Phys. **75**, 403 (2003), J. A. King, et al. MNRAS **422**, 3370 (2012), H. Chand, et al., *Precision Spectroscopy in Astrophysics*]. Important consequences of searching for searching such variations are to establish theories suggesting violation of Einstein's equivalence principle, to support unification of gravity with the other three fundamental interactions of nature [T. Damour, et al., Phys. Rev. D **89**, 081601 (2002), T. Damour, et al., Phys. Rev. D **66**, 046007 (2002), T. Kaluza, Sitzungber. Press. Akad. Wiss. Phys. Math. Kl. L **IV**, 966 (1921), O. Klein, Z. Phys. **37**, 895 (1926), A. Chodos and S. Detweiler, Phys. Rev. D **21**, 2167 (1980), W. J. Marciano, Phys. Rev. Lett. **52**], et cetera. This will also probe the multidimensionality to space as predicted by super-string theories [T. Damour and A. M. Polyakov, Nucl. Phys. B **423**, 532 (1994)]. These theories predict temporal variations of dimensionless fundamental constants including the electromagnetic fine structure constant ($\alpha_e = \frac{e^2}{\hbar c}$) in the low energy limit at the cosmological time-scale.

The primary objective of this thesis is to provide accurate results for the relativistic sensitivity coefficients which can be further used to investigate temporal variation of α_e. We have employed relativistic coupled-cluster (RCC) methods developed by us to determine these sensitivity coefficients in many astrophysically relevant atomic systems and also for some of the atomic clock transitions to study the possible temporal variation of α_e. It can be perceived that the anticipated relativistic effects are quite large in the highly charged ions, and seem to

be the promising candidates for such investigation. So we have considered many possible highly charged ions and investigated enhancement of relativistic effects in these systems. To give more accurate results for the sensitivity coefficients, we also estimate the contributions from the Breit interaction and the dominating quantum electrodynamic (QED) corrections in addition to the contribution from Dirac-Coulomb (DC) Hamiltonian.

For the above purpose, we have developed one-electron detachment and one-electron attachment RCC methods from a closed-shell atomic configurations. Using the above methods, we determine the sensitivity coefficients for three low-lying $3s^23p^5\ ^2P_{3/2} \rightarrow 3s3p^6\ ^2S_{1/2}$, $3s^23p^5\ ^2P_{3/2} \rightarrow 3s3p^6\ ^2S_{1/2}$ and $3s^23p^5\ ^2P_{3/2} \rightarrow 3s^23p^5\ ^2P_{1/2}$ transitions in the Cl-like Mn IX, Fe X, Co XI and Ni XII ions. We also calculate the sensitivity coefficients for the three low-lying transitions $2s^22p^5\ ^2P_{3/2} \rightarrow 2s2p^6\ ^2S_{1/2}$, $2s^22p^5\ ^2P_{3/2} \rightarrow 2s2p^6\ ^2S_{1/2}$ and $2s^22p^5\ ^2P_{3/2} \rightarrow 2s^22p^5\ ^2P_{1/2}$ in the F-like Ti XIV, V XV, Cr XVI, Mn XVII, Fe XVIII, Co XIX, Ni XX, Cu XXI, Zn XXII and Mo XXXIV ions very accurately. In addition to these ions, we have also calculated the sensitivity coefficients for a number of astrophysically relevant transitions in the Si IV, Ti IV and Zn II ions using our RCC methods. Since Si IV, Ti IV and Zn II ions are highly abundant in many quasars, we have provided q-values for a number of important transitions in these ions to achie better statistical analysis in the estimation of α_e variation using the Many-Multiplet (MM) method.

We also carry out very accurate calculations of some of the physical quantities which are vital in the precise estimate of absolute frequencies in the atomic clock experiments. One of them is the quadrupole shift in the Yb^+ ion clock which arises due to the interaction of electric field gradient with the quadrupole moment of the atomic systems. We have investigated quadrupole shifts for three prominent clock transitions, $[4f^{14}6s]^2S_{1/2} \rightarrow [4f^{14}5d]^2D_{3/2}$, $[4f^{14}6s]^2S_{1/2} \rightarrow [4f^{14}5d]^2D_{5/2}$ and $[4f^{14}6s]^2S_{1/2} \rightarrow [4f^{13}6s^2]^2F_{7/2}$, in the Yb^+ ion by calculating quadrupole moments (Θs) of the $[4f^{14}5d]^2D_{3/2,5/2}$ and $[4f^{13}6s^2]^2F_{7/2}$ states using our methods. We find an order difference in the Θ value of the $[4f^{13}6s^2]^2F_{7/2}$ state between our calculation and the experimental result, but our result concur with the other

two calculations that are carried out using different many-body methods than ours. However, our Θ value of the $[4f^{14}5d]^2D_{3/2}$ state is in good agreement with the available experimental result and becomes more precise till date estimating the quadrupole shift of the $[4f^{14}6s]^2S_{1/2} \rightarrow [4f^{14}5d]^2D_{3/2}$ clock transition more accurately.

The other one is the black-body radiation (BBR) shifts due to the magnetic dipole (M1) and electric quadrupole (E2) components of the radiation fields in the Ca^+ and Sr^+ single ion clocks. We have estimated contribution from the M1 and E2 multipoles of the radiation field for the $4s\ ^2S_{1/2} \rightarrow 3d\ ^2D_{5/2}$ and $5s\ ^2S_{1/2} \rightarrow 4d\ ^2D_{5/2}$ transitions in the singly ionized calcium and strontium, respectively. These shifts are obtained by calculating the corresponding multipolar scalar polarizabilities of the involved atomic states. Precise estimate of these systematics are quite important for determining uncertainties to the measured clock frequencies in these ions, which are further used for giving stringent bound on the temporal variation in α_e.

Keywords: Fine structure constant, Sensitivity coefficient, Alkali-Doublet method, Many-Multiplet method, Atomic clock, Dirac-Fock model, Hyperfine interaction, Quadrupole shifts, Black-body radiation shifts, Many-body perturbation theory, Relativistic coupled-cluster method, one-electron detachment method, one-electron attachment method, Ionization potential energies, Electron affinities.

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List of Publications

Publications in journals

1. **D. K. Nandy**, Yashpal Singh, B. K. Sahoo and C. Li, *Sc III spectral properties of astrophysical interest*, J. Phys. B: At. Mol. Opt. Phys. **44**, 225701 (2011).

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6. **D. K. Nandy** and B. K. Sahoo, *Spectral properties of F-like ions*, A&A **563**, A25 (2014).

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10. **D. K. Nandy**, and B. K. Sahoo, *Relativistic calculations of radiative properties and fine structure constant varying sensitivity coefficients in astrophysically relevant Zn II, Si IV, and Ti IV ions*, MNRAS **447**, 3812 (2015).

11. **D. K. nandy**, and B. K. Sahoo, *Forbidden transition properties in the ground-state configurations of singly ionized noble gas atoms for stellar and interstellar media*, MNRAS **450**, 1012 (2015).

12. **D. K. Nandy**, Sukhjit Singh, and B. K. Sahoo, *Radiative properties of few F- and Cl- like alkali and alkaline-earth metal ions*, MNRAS **452**, 2546 (2015).