

## Ab initio multiconfiguration Dirac-Fock calculation of <sup>7</sup>Be to determine the electron density at the nucleus for different electronic configurations and its relation with the electron capture decay rate measurements

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### Introduction

It is known that the electron capture decay rate is directly proportional to the the total electron density nucleus. However the electron density at the nucleus calculated using Wien2K package [1] based on state-of-the art density-functional theory (DFT) showed a very small variation ~0.2% in different environment which cannot explain the large 0.1% to 1.5% change in observed change in electron capture decay rate of <sup>7</sup>Be. Lee et al. [2] employed the Wien2k package for calculating the electron density at the <sup>7</sup>Be in order to understand the variation in electron capture decay rate under compression, found that in comparison to experimental measurements pressure by Hensley et al.[3], calculations for BeO showed results smaller by a factor of 3–6.

In this work, ab-initio, relativistic state-dependent multi-configuration Dirac-Fock (MCDF) calculations have been done for determining the charge density at the nucleus of <sup>7</sup>Be using MCDF program of Grant et al [4] and observed variations in electron density with the configurations considered which reflect different electronic environmental condition in a medium.

### Method of calculation

In order to calculate the electron density at the nucleus, an essential requirement is reliable wave functions. As the MCDF method provides convenient means to include electron correlation and relativity in an integrated way, and produces compact wave functions, we have used this method for determination of electron density at the nucleus. The energy of state  $\alpha$  is

$$E_\alpha = \int \Psi_\alpha^\dagger(\mathbf{r}) H \Psi_\alpha(\mathbf{r}) d\tau \quad (1)$$

where  $H$  is the relativistic N-electron Hamiltonian that can be expressed in second quantised form:  $H =$  (2)

$$\sum N(a_p^\dagger a_q) \langle p | h_D | q \rangle + \frac{1}{2} \sum N(a_p^\dagger a_q^\dagger a_r a_s) \langle pq | R^{-1} + B_T(R) | sr \rangle$$

$N$  represents normal ordering of the creation and annihilation operator enclosed in the brackets. The single-electron Dirac Hamiltonian is given (in au) by

$$h_D = c \vec{\alpha} \cdot \vec{p} + (\beta - 1) c^2 + V_{nuc}(r) \quad (3)$$

where,  $c$  is the velocity of light,  $\vec{\alpha}$  the  $2 \times 2$  pauli matrices,  $\vec{p}$  the momentum operator,  $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ ,

$I$  and  $0$  are the unit respectively zero matrices,  $V_{nuc}(r)$  is the potential due to the nucleus. The inter-electronic separation is denoted by  $R$  and  $B_T(R)$  is the transverse interaction between electrons in the Coulomb gauge derived from the photon propagator in the configuration space in equation (2). In the MCDF-EAL approach, the orbitals are determined self-consistently from an energy functional of the form

$$E = \sum (2J_\alpha + 1) \langle H_c \rangle_{\alpha\alpha} \langle \sum_\alpha (2J_\alpha + 1) \rangle^{-1} \quad (4)$$

where  $H_c$  is the Hamiltonian without the contribution of the Breit interaction. The Breit interaction is considered as a first-order perturbation and evaluated using the techniques given by Grant and McKenzie. Different radial expectation values are determined using following expressions

$$\langle r^k \rangle = \left\langle \Gamma P J M_j \left| \sum_{i=1}^N r_i^k \right| \Gamma P J M_j \right\rangle \quad (5)$$

and electron density at the nucleus using

$$\rho(0) = \left\langle \Gamma P J M_j \left| \sum_{i=1}^N \delta(r_i) \right| \Gamma P J M_j \right\rangle \quad (6)$$

The kinetic energy parameter

$$T = \left( \frac{\Gamma P | M_j}{\int_{\Gamma}^N} [c \alpha_i \cdot p_i + (\beta_i - 1) c^2] \frac{\Gamma P | M_j}{\int_{\Gamma}^N} \right) \quad (7)$$

where  $\frac{\Gamma P | M_j}{\int_{\Gamma}^N}$  represents an eigen state and N is the number of grid points used in the calculation.

### Atomic structure calculation of Beryllium using MCDF

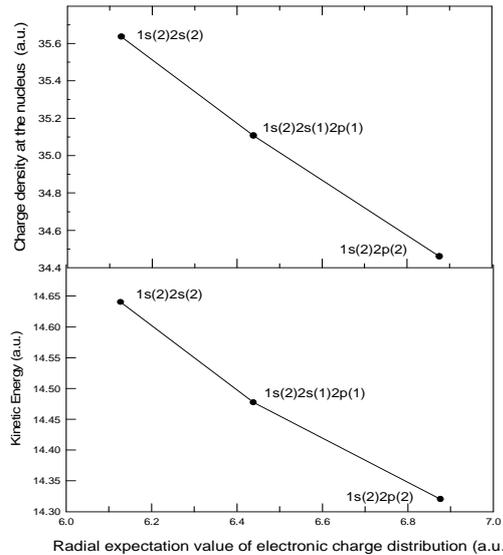
A MCDF wave function for neutral  ${}^7\text{Be}(1s2,2s2)$  and  $\text{Be}(1s2)$ , consisting of *jj* equivalent of a single non-relativistic configuration. In this calculation the nuclear charge density  $\rho_N(\mathbf{r})$  has been modelled with an extended two parameter Fermi distribution [5] and considering  ${}^7\text{Be}$  nucleus, default root mean squared radius = 1.25208 fm and default nuclear skin thickness = 0.52338 fm. Electron charge density  $\rho(\mathbf{0})$  obtained from MCDF calculations for  ${}^7\text{Be}$  having two full 2s electrons (*ns* = 2) is 35.635 and that of a  ${}^7\text{Be}^{++}$  ion, with no 2s electron (*ns* = 0) is 34.602. So the difference of neutral  ${}^7\text{Be}$  atom and  ${}^7\text{Be}^{++}$  ion is 2.9% which is in a reasonably good agreement with the calculations of Hartree and Hartree's 3.31% [5].

Calculations were performed by placing 4 electrons of  ${}^7\text{Be}$  are placed as [1s(2),2s(1),2p(1)], three relativistic CSF (Configuration State functions) based on 4 relativistic subshells are formed. Three atomic levels with J/parity (-1,-1,-2) are optimized considering standard weights. In  $\text{Be}[1s(2),2s(2)]$ ,  $\square=2$  sub-shell was made active and excitations were allowed and thus excited states with 2 electrons occupying p-orbital was constructed. The electron density at the nucleus, radial expectation value and average kinetic energy corresponding to each level were determined.

### Results and conclusion

We find that the electron density at the nucleus for  ${}^7\text{Be}$  varies linearly as 2s electron loses more and more electrons in agreement with our results [6]. We find that as both 2s electrons of  ${}^7\text{Be}$  get excited to 2p orbital, electron density at the nucleus is 34.461, nearly equal to the electron density calculated for  $\text{Be}^{++}$  ion. However we find from Fig 1, the radial expectation value of the electronic distribution and the kinetic energy

increases as  ${}^7\text{Be}$  loses more electron. So,  ${}^7\text{Be}$  is placed in different environment, not only the loss of 2s electrons due to electron affinity of the neighbouring atoms but how far the electron is pulled determines the electron density at the nucleus and we concluded the large variation in observed in the electron capture decay rate of  ${}^7\text{Be}$  can explained based on electron density at the nucleus determined by MCDF calculations.



**Fig. 1** Variation in charge density and average kinetic energy of electrons for different electron configurations with Radial expectation value of electronic charge distribution

### References

- [1] P. Blaha et al., WIEN2k: An Augmented Plane Wave Local Orbitals Program for Calculating Crystal Properties. Technische Universität Wien, Wien, Austria.
- [2] K. K.M. Lee, G. Steinle-Neumann, Earth and Planetary Science Lett. **267** (2008) 628.
- [3] W. K. Hensley, W. A. Bassett, J. R. Huizenga, Science **181** (1973)
- [4] Grant I P and McKenzie B J, J. Phys. B: At. Mol. Phys. **13** (1980) 2671-81, McKenzie B J, Grant I P and Norrington P H 1980 Comput. Phys. Commun. **21** 233-41
- [5] D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) **A150** 9 (1935)
- [6] P. Das and A. Ray, Phys Rev C **71**, 025801 (2005)