Exchange and Overlap Correction for Electron-Capture Decay of Ho

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The exchange and overlap correction factors for electron capture decay probability of Ho atom have been calculated for all s and p electrons by the use of the Dirac-Fock wave functions. The effect of the presence of a vacancy in the daughter atom as a consequence of electron capture is taken into consideration. The results are compared with other calculations and the values with the Dirac-Fock-Slater wave functions.

KEY WORDS: Exchange and Overlap Correction/ Electron-Capture Decay/ Ho Atom/

I. INTRODUCTION

In the simple theory of electron-capture decay, the probability that an electron is captured by the nucleus is described only in terms of the wave function of this electron at the position of the nucleus. However, owing to the lack of orthogonality of the atomic wave functions between the initial and final states due to the change in atomic potential, the existence of other electrons should be taken into account in the complete description of nuclear electron-capture process. This is well known as the exchange and overlap effects in electron capture.

Benoist-Gueutal[1] first suggested the importance of the effect of imperfect overlap of the atomic wave functions. She showed that this effect almost doubles the L/K capture ratio for [7]Be. A similar calculation for [37]Ar has been made by Odiot and Daudel.[3] Their results are in agreement with the experimental value for the L/K capture ratio of this nuclide.

A systematic study of the role of atomic electrons in the nuclear electron-capture decay process has been made by Bahcall,[3] using the ground-state wave function for the initial and final atomic states. He derived a simple formula for the exchange and overlap corrections in electron-capture probability. Subsequently Vatai[4] pointed out the importance of the presence of an inner-shell vacancy in the daughter atom produced by electron capture. He obtained another expression for the exchange and overlap correction factor. Later works on the exchange and overlap corrections in electron-capture decay using various atomic wave functions in both correction formulas are summarized in the recent review article.[5]

The difference between the correction factors obtained by Bahcall and by Vatai is understood to consist in the different approach to treat the shakeoff process, in which

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another atomic electron in the same atom is ejected into the continuum in the final state by the sudden change in the central potential due to electron capture of an inner-shell electron. At present both correction factors have been used to take into account the exchange and overlap effects. In general, the Vatai correction underestimates the L/K capture ratio, but agrees with the measured values for the M/L ratios. On the other hand, the Bahcall correction is in better agreement with the experimental L/K capture ratios.

The similar exchange and overlap effects have also been known when an inner-shell vacancy is created and studied for the case of x-ray intensity ratios,[6] photoelectric effect[7] and internal conversion.[8]

Recently [163]Ho nuclide has received a special interest as the most promising nuclide to measure the rest mass of electron neutrino and extensive experimental studies on the electron capture decay of this nuclide have been made.[9-12] The Q value of this nuclide for electron capture decay is known to be $2.70^{+0.13}_{-0.002}$ keV.[13] Owing to the smallness of the Q value, the ground state of [163]Ho can decay to the ground state of [163]Dy through M- and higher-shell electron capture. In order to determine the rest mass of the electron neutrino, it is important to estimate the exchange and overlap effects for M- and outer-shell capture accurately. However, for some outer-shell electrons, the exchange and overlap correction factors are unknown for electron-capture decay of Ho. Especially, there have been reported no theoretical calculations for the $3p_{1/2}$, $4p_{1/2}$, and $5p_{1/2}$ shells.

It is the purpose of the present work to calculate the exchange and overlap correction factors for all s- and $p_{1/2}$-shell electrons for electron-capture decay of holomium atom. The calculations have been made in the Bahcall and Vatai models by the use of the Dirac-Fock (DF) wave functions. The presence of a vacancy in the daughter atom due to electron capture and the effect of the finite nuclear size are taken into consideration. For comparison, the correction factors have also been obtained with the Dirac-Fock-Slater (DFS) wave functions. The calculated results are compared with other existing theoretical calculations.

II. THEORETICAL MODELS

According to the usual theory of orbital electron capture, the probability that an electron is captured by the nucleus is written by[5]

$$\lambda = \frac{G^2 \xi}{2\pi} \sum_i q_i^2 B_i |\psi_i(0)|^2 , \qquad (1)$$

where G is the β-decay coupling constant, ξ is the appropriate combination of nuclear matrix elements, q_i is the energy of the neutrino which is emitted during the i-shell electron capture, B_i is the exchange and overlap correction factor for the i-shell capture, and $\psi_i(0)$ is the i-shell electron wave function of the parent atom at the nuclear surface. Here we assume that the rest mass of the electron neutrino is negligibly small.

In order to avoid the summation over the infinite number of possible final atomic

states, Bahcall[3] made the simplifying assumptions, which were discussed in Ref. 5. He treated that the outer-shell electron states form practically a complete set and neglected the contributions from the electrons outside the $3s$ shell. This approximation is useful for inner-shell electron capture because it partially takes into account the shakeoff and shakeup processes.

According to the Bahcall theory, the exchange and overlap correction factor is given by

$$B_i = |f_i/\psi_i(0)|^2. \tag{2}$$

The capture amplitude f_i, for example, for the $3s$ capture is expressed as

$$f_{3s} = \langle 1s' | 1s \rangle \langle 2s' | 2s \rangle \psi_{3s}(0) - \langle 1s' | 3s \rangle \langle 2s' | 2s \rangle \psi_{1s}(0)$$
$$- \langle 2s' | 3s \rangle \langle 1s' | 1s \rangle \psi_{2s}(0) , \tag{3}$$

where $|1s\rangle$ means the $1s$-shell wave function in the parent atom and the primed orbitals pertain to the daughter atom. The capture amplitudes for other orbitals can be defined in the similar manner.

In the original Bahcall theory, the overlap integral $\langle ns' | ns \rangle$ in Eq. (3) was obtained by the use of the ground-state wave functions for the parent and daughter atoms and the presence of the vacancy was not taken into account. However, Vitai[4] showed that the inner-shell vacancy in the daughter atom plays an important role for the B_i factor.

In the present work, we introduce two modifications to the Bahcall theory. First, all the atomic shells up to $n=5$ are included in Eq. (3), where n is the principal quantum number. This is because we are interested in the outer-shell electron capture. Second, the existence of the vacancy in the daughter atom is taken into consideration. Hereafter, we call this model as the Bahcall correction.

On the other hand, neglecting the process involving shakeoff and shakeup, Vatai[4] calculated the exchange and overlap correction factors by the use of many-electron wave functions. He retained only the exchange integral in the form of $\langle \psi_{\beta'} | \psi_i \rangle$ and neglected all other exchange integrals $\langle \psi_{\beta'} | \psi_\beta \rangle$ for $\beta' \neq \beta$. His expression for the capture amplitude is in the following form:

$$f_{3s} = \psi_{3s}(0) \langle 1s' | 1s \rangle \langle 2s' | 2s \rangle \langle 2p' | 2p \rangle \cdots$$
$$- \psi_{1s}(0) \langle 1s' | 3s \rangle \langle 2s' | 2s \rangle \langle 2p' | 2p \rangle \cdots$$
$$- \psi_{2s}(0) \langle 1s' | 1s \rangle \langle 2s' | 3s \rangle \langle 2p' | 2p \rangle \cdots$$
$$- \cdots\cdots\cdots\cdots\cdots . \tag{4}$$

In Eq. (4), the presence of the hole in the daughter atom is considered. We call this model as the Vatai correction.

III. RESULTS AND DISCUSSION

All the calculations in the present work have been performed on the FACOM R-382 computer in the Data Processing Center of Kyoto University. The atomic

wave functions have been obtained with the DF method.[12] The initial state corresponds to the ground state of Ho atom, while the final state is the Dy atom in the electronic configuration of Ho with a vacancy. The correction factors have been calculated according to the Bahcall and Vatai corrections.

The effect of finite nuclear size is taken into account by assuming that the proton charge distribution in the nucleus is given by the Fermi distribution. The values of wave functions at the nuclear surface are in good agreement with the tabulated values of Mann and Waber.[15] In order to test the effect of the charge distribution, the calculations with the assumption that the nucleus is expressed as a uniformly charged sphere have been made. The correction factors obtained with both distributions agree well with each other.

The calculated results are shown in Table I. In general, the values based on the Vatai correction are somewhat smaller than those from the Bahcall correction, but both results are in good agreement with each other.

Table I. Comparison of exchange and overlap correction factor for electron capture decay of Ho atom.

Shell	MB[a]	Bennett[b]	DFS		DF	
			B[c]	V[d]	B	V
K	0.992		0.993	0.993	0.990	0.989
L_1	1.026		1.033	1.031	1.031	1.030
L_2	0.989		0.989	0.986	0.981	0.979
M_1	1.063	1.065	1.089	1.081	1.086	1.083
M_2		0.935	1.039	1.030	1.035	1.031
N_1		1.12	1.166	1.152	1.159	1.151
N_2		0.88	1.121	1.107	1.116	1.108
O_1		1.18	1.225	1.217	1.265	1.248
O_2		0.82	1.257	1.225	1.247	1.224

a) Martin and Blichert-Toft (Ref. 17).
b) Bennett (Ref. 18).
c) Bahcall correction.
d) Vatai correction.

It is also clear from the table that the correction factor becomes larger for outer-shell electrons. This can be understood as follows. For inner-shell electron capture, the outer-shell electron feels the decrease in the nuclear charge by electron capture and the decrease in the screening effect due to sudden loss of the captured electron. Both effects cancel with each other and the effective nuclear charge seen by this electron does not change during electron-capture decay. Then the exchange effect for outer-shell electrons can be neglected because of orthogonality of the atomic wave functions between the initial and final states. The B_i factor is mainly ascribed to the inner-shell electrons, as assumed by Bahcall. On the other hand, in the case of the outer-shell electron capture, the inner-shell electrons experience the change in the nuclear charge and the outer-shell electrons feel the change in the central potential due to the presence of the vacancy.

For comparison, the results obtained with the DFS wave functions[16] are also listed in the table. In the DFS model, the statistical scaling parameter α is set to be unity. The DFS results are in agreement with the DF ones. This fact suggests that the wave-function effect is not important.

The present results are compared with other theoretical calculations. All the previous calculations for the exchange and overlap correction factors have been compiled and compared in detail by Bambynek et al.[5] Only one calculation for electron-capture decay of Ho atom has been reported.[17] Martin and Blichert-Toft calculated the correction factors for K, L_1, $L_{2,3}$, and M_1 shells in the Vatai's approach, using the DFS wave functions. Their values for the K and L_2 shells are a little larger than the present ones, but those for the L_1 and M_1 shells are smaller. However, it can be said that agreement between two calculations is good.

Bennett[18] estimated the correction factors for the M_1, N_1, and O_1 shells, based on interpolation and extrapolation of the values from the table of Bambynek et al.[5] For the M_2, N_2, and O_2 shells, he assumed that the average of ns and $np_{1/2}$ factors is unity. His values for the ns shells are in agreement with the present results. However, for the $np_{1/2}$ shells the values of Bennett are smaller than unity, while the values obtained in the present work are larger than unity. This fact indicates that the assumption made by Bennett is invalid.

In conclusion, the exchange and overlap correction factors for electron-capture decay of Ho atom have been calculated with the DF wave functions. The obtained results are in agreement with other theoretical calculations, except for the assumed values of Bennett for the outer $np_{1/2}$ shells. The present correction factors are useful to estimate the rest mass of the electron neutrino by the use of electron-capture decay of ^{163}Ho.

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