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Atomic Electron Correlation in Nuclear Electron Capture

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The effect of electron-electron Coulomb correlation on orbital electron capture by the nucleus has been treated by the multiconfigurational Hartree-Fock approach. The theoretical ^{7}Be L/K capture ratio is found to be 0.086, and the ^{37}Ar M/L ratio, 0.102. Both ratios are smaller than the independent-particle predictions. Measurements exist for the Ar M/L ratio, and agreement between theory and experiment is excellent.

Benoist-Gueutal's insight[1] that atomic electrons must be included in a complete description of orbital electron capture by the nucleus[2] led to the introduction of atomic exchange and imperfect-overlap factors in the theoretical capture probability.[3-6] All existing work on electron capture has been carried out in the independent-particle approximation; effects due to electron-electron Coulomb correlation have been neglected. Here we report on a first effort to take correlation into account, by using the multi-configurational Hartree-Fock (MCHF) approach.[7] We calculate the ^{7}Be L/K and ^{37}Ar M/L capture ratios.

The nuclear electron capture rate is[2]

$$\lambda_i = \lambda_i^0 B_i, \quad i = K, L, M, \ldots, \tag{1}$$

where λ_i^0 is the rate obtained when atomic matrix elements are neglected,[8] and B_i is the exchange-overlap correction factor. For example, if the initial and final states are represented by a single Slater determinant, B_K is

$$B_K = K\{\langle 2s'|2s\rangle\langle 3s'|3s\rangle - \langle 2s'|1s\rangle\langle 3s'|3s\rangle[R_{2s}(0)/R_{1s}(0)] - \langle 2s'|2s\rangle\langle 3s'|1s\rangle[R_{3s}(0)/R_{1s}(0)]\}^2, \tag{2}$$

where

$$K = \langle 1s'|1s\rangle^2\langle 2s'|2s\rangle^2\langle 2p'|2p\rangle^{2q(2p)}\langle 3s'|3s\rangle^{2[q(3s)-1]}\langle 3p'|3p\rangle^{2q(3p)}. \tag{3}$$

Here, $q(n\ell)$ is the occupation number of the $n\ell$ shell, and primes denote the daughter atom. Bahcall[2-6] set K=1, while Vatai[2,9] retained the factor. Similar expressions exist for B_L and B_M.

The capture ratio for shells i and j, in allowed transitions, is[2]

$$(\lambda_i/\lambda_j) = (\lambda_i/\lambda_j)^0 (B_i/B_j), \qquad (4)$$

where

$$(\lambda_i/\lambda_j)^0 = [R_i^2(0)/R_j^2(0)](q_i^2/q_j^2), \quad i, j = K, L_1, M_1. \qquad (5)$$

The R's are electron radial wave functions, evaluated at the origin, and the q's are neutrino energies. The contributions from L_2 and M_2 electrons are neglected here.

In our MCHF calculation, the ground state is

$$\Psi_g(\gamma LS) = \sum_i C_i \; \Phi(\gamma_i LS) \qquad (6)$$

and the final-state wave function, describing the hole state after capture, is

$$\Psi_j'(\gamma LS) = \sum_i C_{ji}' \; \Phi_i'(\gamma_i LS). \qquad (7)$$

The atomic matrix elements become

$$\langle \Psi_j | \mathcal{O} | \Psi_g \rangle = \sum_{i,k} C_{jk}' C_i \langle \Phi_k' | \mathcal{O} | \Phi_i \rangle, \qquad (8)$$

where we have $\mathcal{O} = \sum_b a_b R_b(0)$, and a_b is the destruction operator.[4] The exchange-overlap correction factor is

$$B_i = \sum_j \left| \frac{\langle \Psi_j | \mathcal{O} | \Psi_g \rangle}{R_i(0)} \right|^2 , \qquad (9)$$

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where the summation extends over the states included in the multi-configurational expansion.

For the ^{7}Be L/K capture-ratio calculation, the ground state is represented by

$$\Psi_g = C_1\Phi_1\ (1s^2 2s^2) + C_2\Phi_2(1s^2 2p^2). \tag{10}$$

The 1s-hole state after K capture is

$$\Psi_j = C'_{j1}\Phi'_1(1s2s^2) + C'_{j2}\Phi'_2(1s2p^2). \tag{11}$$

The 2s-hole state after L_1 capture is represented by the single configuration

$$\Psi_j = \Phi'(1s^2 2s). \tag{12}$$

For the ^{37}Ar M/L capture-ratio calculation, we take the ground-state MCHF wave function to be

$$\begin{aligned}\Psi_g = {} & C_1\Phi_1(1s^2 2s^2 2p^6 3s^2 3p^6) \\ & + C_2\Phi_2\left(1s^2 2s^2 2p^6 3p^6 3d^2\ ({}^1S)\right) \\ & + C_3\Phi_3\left(1s^2 2s^2 2p^6 3s^2 3p^4({}^1S)3d^2({}^1S)\right) \\ & + C_4\Phi_4\left(1s^2 2s^2 2p^6 3s^2 3p^4({}^3P)3d^2({}^3P)\right) \\ & + C_5\Phi_5\left(1s^2 2s^2 2p^6 3s^2 3p^4({}^1D)3d^2({}^1D)\right).\end{aligned} \tag{13}$$

The 2s-hole state is

$$\begin{aligned}\Psi_j = {} & C_{j1}\Phi'_1(1s^2 2s2p^6 3s^2 3p^6) \\ & + C_{j2}\Phi'_2\left(1s^2 2s2p^6 3s^2 3p^4({}^1S)3d^2({}^1S)\right) \\ & + C_{j3}\Phi'_3\left(1s^2 2s2p^6 3s^2 3p^4({}^3P)\,{}^4P3d^2({}^3P)\right) \\ & + C_{j4}\Phi'_4\left(1s^2 2s2p^6 3s^2 3p^4({}^3P)\,{}^2P3d^2({}^3P)\right) \\ & + C_{j5}\Phi'_5\left(1s^2 2s2p^6 3s^2 3p^4({}^1D)3d^2({}^1D)\right).\end{aligned}$$

The 3s-hole state after M_1 capture is

$$\begin{aligned}\Psi_j = {} & C_{j1}\Phi_1' \ (1s^2 2s^2 2p^6 3s 3p^6) \\ & + C_{j2}\Phi_2' \left(1s^2 2s^2 2p^6 3s^2 3p^4 ({}^1D) 3d\right) \\ & + C_{j3}\Phi_3' \left(1s^2 2s^2 2p^6 3s 3p^4 ({}^1S) 3d^2 ({}^1S)\right) \\ & + C_{j4}\Phi_4' \left(1s^2 2s^2 2p^6 3s 3p^4 ({}^3P)\, {}^4P\, 3d^2 ({}^3P)\right) \\ & + C_{j5}\Phi_5' \left(1s^2 2s^2 2p^6 3s 3p^4 ({}^3P)\, {}^2P\, 3d^2 ({}^3P)\right). \end{aligned} \qquad (15)$$

The MCHF wave functions were computed with the Froese-Fischer program.[7] The electrostatic interaction matrix elements were calculated with Hibbert's program.[10] The one-electron overlap integrals are listed in Tables I and II. The electron radial-wave-function ratios at the origin and the overlap-exchange correction factors B_i as well as the electron-capture ratios are listed in Table III. For comparison, theoretical single-configuration HF capture ratios[2] and the experimental result[11] for ^{37}Ar are also listed; there is no measurement of the ^7Be L/K ratio.

Electron correlation is seen to have a substantial effect on nuclear capture ratios when outer electrons are involved. Compared with single-configuration HF results according to Vatai's approach,[2] the MCHF L/K capture ratio of ^7Be is reduced by 4.4%; the ^{37}Ar M/L ratio is reduced by 11% and brought into excellent agreement with experiment.[2,11]

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TABLE I. MCHF $\langle n\ell' | n\ell \rangle$ overlap integrals for $_4$Be electron capture

	K capture			L_1 capture	
	$|1s\rangle$	$|2s\rangle$	$|2p\rangle$	$|1s\rangle$	$|2s\rangle$
$\langle 1s'|$	0.97209	-0.19099		0.96247	-0.15591
$\langle 2s'|$	0.17193	0.96785		0.08271	0.88283
$\langle 2p'|$			0.99260		

TABLE II. MCHF $\langle n\ell' | n\ell \rangle$ overlap integrals for $_{18}$Ar electron capture

	$\|1s\rangle$	$\|2s\rangle$	$\|2p\rangle$	$\|3s\rangle$	$\|3p\rangle$	$\|3d\rangle$
L_1 capture						
$\langle 1s' \|$	0.99873	-0.02977		-0.00630		
$\langle 2s' \|$	0.02705	0.99250		-0.10496		
$\langle 2p' \|$			0.99858		-0.02279	
$\langle 3s' \|$	0.00798	0.10177		0.99274		
$\langle 3p' \|$			0.02142		0.99927	
$\langle 3d' \|$						0.99954
M_1 capture						
$\langle 1s' \|$	0.99875	-0.02921		-0.00628		
$\langle 2s' \|$	0.02623	0.99228		-0.09736		
$\langle 2p' \|$			0.99445		-0.08177	
$\langle 3s' \|$	0.00702	0.09020		0.98913		
$\langle 3p' \|$			0.07552		0.99047	
$\langle 3d' \|$						0.93200

TABLE III. Electron radial wave-function ratios $R^2_{ns}(0)/R^2_{n's}(0)$, exchange-overlap correction factors B_i and capture ratios λ_i/λ_j.

Element	Quantity		Result
$^{7}_{4}Be$	$R^2_{2s}(0)/R^2_{1s}(0)$	HF	0.0332
		MCHF[c]	0.0300
	B_K	HF(V)[a]	0.816
		HF(B)[b]	0.900
		MCHF[c]	0.792
	B_L	HF(V)[a]	2.222
		HF(B)[b]	3.045
		MCHF[c]	2.259
	λ_L/λ_K	HF(V)[a]	0.090
		HF(B)[b]	0.112
		MCHF[c]	0.086
$^{37}_{18}Ar$	$R^2_{3s}(0)/R^2_{2s}(0)$	HF	0.0977
		MCHF[c]	0.0669
	B_L	HF(V)[a]	1.121
		HF(B)[b]	1.171
		MCHF[c]	1.098
	B_M	HF(V)[a]	1.322
		HF(B)[b]	1.549
		MCHF[c]	1.674
	λ_M/λ_L	HF(V)[a]	0.115
		HF(B)[b]	0.129
		MCHF[c]	0.102
		Experiment[d]	$0.104^{+0.007}_{-0.003}$

Footnotes to Table III.

[a]Hartree-Fock, Vatai's approach (Refs. 2,9).

[b]Hartree-Fock, Bahcall's approach (Refs. 2, 3-6).

[c]Present multi-configurational HF calculation.

[d]Ref. 11.