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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]

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

where

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

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

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

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

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

The atomic matrix elements become

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

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

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

where the summation extends over the states included in the multiconfigurational 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

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

The 3s-hole state after M_1 capture is

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

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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[1]P. Benoist-Gueutal, C. R. Acad. Sci (Paris) 230, 624 (1950).

[2]For a recent review, see W. Bambynek, H. Behrens, M. H. Chen, B. Crasemann, M. L. Fitzpatrick, K. W. D. Ledingham, H. Genz, M. Mutterer, and R. L. Intemann, Rev. Mod. Phys. 49, 78 (1977).

[3]J. N. Bahcall, Phys. Rev. Lett. 9, 500 (1962).

[4]J. N. Bahcall, Phys. Rev. 129, 2683 (1963).

[5]J. N. Bahcall, Phys. Rev. 131, 1756 (1963).

[6]J. N. Bahcall, Nucl. Phys. 71, 267 (1965).

[7]C. Froese-Fischer, Comp. Phys. Comm. 4, 107 (1972).

[8]H. Brysk and M. E. Rose, Rev. Mod. Phys. 30, 1169 (1958).

[9]E. Vatai, Nucl. Phys. A156, 541 (1970).

[10]A. Hibbert, Comp. Phys. Comm. 2, 180 (1971).

[11]J. P. Renier, H. Genz, K. W. D. Ledingham, and R. W. Fink, Phys. Rev. 166, 935 (1968).

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_4Be	$R^2_{2s}(0)/R^2_{1s}(0)$	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.