surement at 20 keV, our total integrated current density was less than that at which a 1% change in yield was observed.

ACKNOWLEDGMENT

The authors express their gratitude to D. L. Potter, R. D. Worley, N. T. Olson, R. G. Musket, and W. Siekhaus for many helpful suggestions. Fellowships from the National Science Foundation and the Atomic Energy Commission through the Oak Ridge Associated Universities are gratefully acknowledged (RRH and FWR).

*This work was partially supported by the NASA Lewis Research Center.

†Present address: Hughes Research Laboratories, Malibu, California.

[1]E. Merzbacher and H. W. Lewis, Encyclopedia of Physics, edited by S. Flügge (Springer-Verlag, Berlin, 1958).

[2]J. M. Khan, D. L. Potter, and R. D. Worley, Phys. Rev. 139, 1735 (1965).

[3]S. K. Allison and S. D. Warshaw, Rev. Mod. Phys. 25, 779 (1953).

[4]L. C. Northcliffe, Ann. Rev. Nucl. Sci. 13, 67 (1963).

[5]R. R. Hart, N. T. Olson, Harold P. Smith, Jr., and J. M. Khan, J. Appl. Phys. 39, 5538 (1968).

[6]J. H. Ormrod and H. E. Duckworth, Can. J. Phys. 41, 1424 (1963).

[7]R. W. Fink, R. C. Jopson, Hans Mark, and C. D. Swift, Rev. Mod. Phys. 38, 513 (1966).

[8]M. C. Walske, Phys. Rev. 101, 940 (1956).

[9]W. Primak and J. Luthra, J. Appl. Phys. 37, 2287 (1966).

PHYSICAL REVIEW VOLUME 179, NUMBER 1 5 MARCH 1969

Radiative Decay Rates of Vacancies in the K and L Shells*

James H. Scofield

Lawrence Radiation Laboratory, University of California, Livermore, California 94550

(Received 6 December 1968)

A calculation is made of the rates of emission of x rays in the filling of vacancies in the K and L shells. The total radiative decay rates and the rates of emission of a number of x-ray lines are presented for a range of elements. The atomic electrons are taken to be in single-particle states in a central potential given by the relativistic Hartree-Slater theory. All multipoles of the radiation field and all transitions from occupied states of the atom are included. The electrons are treated relativistically and the effect of retardation is included.

INTRODUCTION

A vacancy in one of the levels of an atom may be filled by an electron from a higher level accompanied by the ejection of either a second electron or an x ray. This paper gives the results of a calculation of the rate of decay of vacancies in the K and L shells accompanied by the radiation of x rays. In the calculation, the electrons are treated relativistically and the effect of retardation is included. The electrons are treated as moving independently with their mutual interactions accounted for by a central potential. The potential used is one given by the Hartree-Slater theory.

Relativistic calculations of the radiative transition rates have previously been carried out by Massey and Burhop,[1] Laskar,[2] Payne and Levinger,[3] Asaad,[4] Taylor and Payne,[5] and Babushkin.[6] All of these calculations except Asaad's are based on the Coulomb potential. Massey and Burhop, Laskar, and Babushkin introduced an effective nuclear charge to account for the screening of the nucleus by the electrons. Asaad's calculation is based on a more realistic potential obtained from a self-consistent field calculation. The calculations of Massey and Burhop, Laskar, and Asaad do not include the effect of retardation; i.e., they assume the x ray's wavelength is much greater than the atomic dimensions. The inclusion of retardation is incorrect in the work of Payne and Levinger and Taylor and Payne. Babushkin

includes retardation; he gives the theoretical formulas for all the multipoles and numerical results for a Coulomb potential for the L_I to K $M1$ transition and the $E1$ transitions to the K shell.

EMISSION OF MULTIPOLE RADIATION BY ELECTRONS

The radiative transition rate for an electron to go from a state a to a state b with the emission of photons of energy ω and momenta $\vec{k}$ is given by[7]

$$\Gamma_{ab} = (\alpha\omega/2\pi)\sum_{\text{pol}} \int d\Omega_k \, |\, (b\,|\,\vec{\alpha}\cdot\vec{\epsilon}_r^{\,*} e^{-i\vec{k}\cdot\vec{r}}\,|\,a)\,|^2$$

with $\hbar = c = m_e = 1$.

In terms of the multipole fields, the rate is given by

$$\Gamma_{ab} = 4\pi^2\alpha\omega \sum_{L=1}^{\infty} \sum_{M=-L}^{L} [\,|(b\,|\,\vec{\alpha}\cdot\vec{A}_{LM}(m)\,|\,a)|^2 + |(b\,|\,\vec{\alpha}\cdot\vec{A}_{LM}(e)\,|\,a)|^2],$$

with the magnetic and electric multipoles normalized to

$$\vec{A}_{LM}(m) = i(2/\pi)^{1/2} j_L(kr)[L(L+1)]^{-1/2}\,\vec{L}\,Y_{LM}(\hat{r}),$$

$$A_{LM}(e) = (2/\pi)^{1/2} k[L(L+1)]^{-1/2}\,\vec{\nabla}\times\vec{L} j_L(kr) Y_{LM}(\hat{r}), \quad \text{where} \quad \vec{L} = -i\vec{r}\times\vec{\nabla}.$$

The equality of the two expansions is presented by Rose,[8] while a development directly in terms of the multipole fields is given by Moszkwoski.[9]

We may simply follow the work of Rose *et al.*[10] on internal conversion to obtain the expression for the transition rate between single-particle electron states in a spherically symmetric potential in terms of the radial wave functions.

We have, after averaging over the magnetic quantum numbers of the final state,[11]

$$\Gamma_{ab} = 2\alpha\omega^2 \sum_L [f_L(m) + f_L(e)],$$

with $f_L(m) = \omega^{-1} B(-\kappa_a, \kappa_b, L) R_L^{\,2}(m)$, $f_L(e) = \omega^{-1} B(\kappa_a, \kappa_b, L) R_L^{\,2}(e)$,

$$B(\kappa_a, \kappa_b, L) = [(2l_a+1)(2l_b+1)/L(L+1)]\; C^2(l_a, l_b, L; 0, 0) W^2(j_a l_a j_b l_b; \tfrac{1}{2} L).$$

The eigenvalues κ_a and κ_b distinguish the initial and final angular momentum states. The total angular momentum j and the dominant orbital angular moment l are related to the κ by

$$j = |\kappa| - \tfrac{1}{2}, \quad l = \kappa \text{ for } \kappa \text{ positive}, \quad l = -\kappa - 1 \text{ for } \kappa \text{ negative}.$$

The quantity $B(\kappa_a, \kappa_b, L)$ is zero unless the sum $J = L + l_a + l_b$ is even and L, j_a, j_b form a triangle. When these conditions are met, we have[12]

$$C^2(l_a, l_b, L; 0, 0) = \frac{(2L+1)\,(J-2L)!\,(J-2l_a)!\,(J-2l_b)!}{(J+1)!} \left(\frac{(J/2)!}{(J/2-L)!\,(J/2-l_a)!\,(J/2-l_b)!} \right)^2,$$

and $W^2(j_a l_a j_b l_b; \tfrac{1}{2} L) = \left| (L + \kappa_a + \kappa_b + 1)(\kappa_a + \kappa_b - L)/4\kappa_a\kappa_b(2\kappa_a+1)(2\kappa_b+1) \right|$.

The radial matrix elements are given by

$$R_L(m) = (\kappa_a + \kappa_b) \int dr\, j_L(kr)(F_b G_a + G_b F_a),$$

$$R_L(e) = \int dr \{ j_{L-1}(kr)[(\kappa_b - \kappa_a)(F_b G_a + G_b F_a) + L(F_b G_a - G_b F_a)] + L(G_b G_a + F_b F_a) j_L(kr) \}.$$

Alternatively,

$$R_L(e) = \int (dr/kr)[(F_b G_a - G_b F_a)L(L+1)j_L(kr) + (\kappa_b - \kappa_a)(F_b G_a + G_b F_a)(r\,d/dr + 1)j_L(kr)] .$$

The F and G here include a factor of r and are normalized by

$$\int dr(F^2 + G^2) = 1.$$

They satisfy the energy eigenvalue equations

$$(d/dr + \kappa/r)G = (E - V + 1)F, \quad (-d/dr + \kappa/r)F = (E - V - 1)G.$$

The total radiative decay rate of a vacancy in the state b is given by summing the transition rates to the state b of all of the electrons with single-particle energies greater than that of the state b. Each energy level is occupied by at most $2j_a + 1$ electrons.

THE CALCULATION

The potential used for the calculation is the relativistic version of the potential used by Herman and Skillman[13] and was introduced in relativistic calculations by Liebermann, Waber, and Cromer.[14] Slater's correction term for the effect of exchange,

$$V_S = -1.5e^2(3\rho/\pi)^{1/3},$$

where ρ is the electron density, is added to the potential due to the electron and nuclear charges. The modification due to Latter is used in that the potential is set equal to $-e^2/r$ in the outer region in which it would otherwise rise above this in value.

The atomic ground-state configurations used are those as listed by Foster.[15] For the partially filled outer levels with greater than zero orbital angular momentum, the electrons have been proportioned between the two levels differing only in their total angular momentum according to the statistical weights of the two levels.

An iterative procedure is used to find the potential arising from the occupation of the single-particle levels in the potential by the specified number of electrons. The radial matrix elements for the allowed transitions are then found by integrating the products of the initial and final wave functions and the spherical Bessel functions.

The results for the total radiative decay rates and the emission rates for the stronger x-ray lines are listed in Tables I through IV for vacancies respectively in the $K, L_{\mathrm{I}}, L_{\mathrm{II}}$, and L_{III} levels. Checks of the results set the inaccuracies due to the numerical integrations at or less than 0.1%.

An estimate of the accuracy of the model is obtained by comparing the experimental and calculated values for the electron binding energies and x-ray energies. Assuming the errors in the energies are due to errors in the potential, we calculate the amount such a change in the potential will vary the transition rates. As pointed out by Manson and Cooper,[16] the transition rates are sensitive to the normalization near the origin of the upper state, particularly for states near the ionization limit. If we fix the normalization of the wave functions near the origin and take out the factor for the normalization, the remaining factor is relatively insensitive to variations in the potential or the binding energy even from one shell to the next for a given value of κ. We consider the normalization factor to be a function of the binding energy of the upper state and the remaining factor a function of the x-ray energy. The variation of these two factors was obtained by using a potential which had not relaxed to its self-consistent value. The experimental values of the energies were obtained from the listing of Bearden and Burr[17] with an allowance of 7 eV for the Fermi energy.[18] The estimated errors in the transition rates are listed in Table V for the E1 transition. The errors in the other multipoles examined were at most only slightly larger.

For the lower atomic numbers, the inaccuracies in the energies and the transition rates come from inaccuracies in the description of the interaction between the electrons. For the large atomic numbers, relativistic effects further modify the interaction between the electrons and, in addition, corrections enter from the quantization of the radiation field and from the penetration of the electrons into the nucleus.[19]

For each transition of an electron from an occupied level to the one with a vacancy, the rates of emission of all the allowed multipoles of the radiation field were calculated. Only the $E1, E2, M1$, and $M2$ transitions give any significant contribution to the total decay rates. In Table VI are listed the contributions of each of the multipoles to the total radiative decay rate for the K shell in uranium ($Z = 92$). In Table VII are listed the total f values and decay rates for all of the transitions from the different levels of the N shell to the K shell.

In the nonrelativistic limit with no retardation, the nonvanishing of the magnetic dipole transition

TABLE I. Calculated K x-ray emission rates, in units of (eV/$\hbar$).

Element	Z	Total	L_{I} $2s_{1/2}$	L_{II} $2p_{1/2}$	L_{III} $2p_{3/2}$	M_{II} $3p_{1/2}$	M_{III} $3p_{3/2}$	M_{IV} $3d_{3/2}$	M_{V} $3d_{5/2}$	N_{II} $4p_{1/2}$	N_{III} $4p_{3/2}$	$N_{\mathrm{IV,\,V}}$ $4d_{3/2,\,5/2}$	$O_{\mathrm{II,\,III}}$ $5p_{1/2,\,3/2}$
Al	13	0.0138		0.0046	0.0091								
S	16	0.0398		0.0128	0.0253	0.000 60	0.001 18						
Ar	18	0.0717		0.0223	0.0440	0.001 82	0.0036						
Ca	20	0.1194		0.0363	0.0716	0.003 86	0.0076						
Ti	22	0.1860		0.0563	0.1107	0.0064	0.0126						
Mn	25	0.332		0.1003	0.1967	0.0119	0.0235						
Fe	26	0.396		0.1196	0.2341	0.0144	0.0283						
Cu	29	0.642		0.1942	0.379	0.0235	0.0460						
Zn	30	0.747		0.2254	0.439	0.0279	0.0545						
Ge	32	0.996		0.2990	0.580	0.0387	0.0755			0.000 63	0.001 21		
Kr	36	1.686		0.499	0.961	0.0702	0.1368	0.000 20	0.000 29	0.0062	0.0119		
Rb	37	1.905		0.562	1.080	0.0805	0.1570	0.000 26	0.000 37	0.0084	0.0163		
Zr	40	2.688		0.786	1.504	0.1186	0.2310	0.000 49	0.000 70	0.1060	0.031		
Mo	42	3.33		0.970	1.848	0.1505	0.2930	0.000 73	0.001 03	0.0218	0.042		
Ag	47	5.42		1.571	2.961	0.2582	0.5017	0.001 75	0.002 44	0.043	0.083	0.000 47	
Sn	50	7.09	0.000 127	2.047	3.83	0.346	0.671	0.002 77	0.003 84	0.063	0.121	0.000 97	0.0040
Sb	51	7.72	0.000 157	2.228	4.16	0.379	0.735	0.003 21	0.0044	0.070	0.136	0.001 21	0.0082
Ba	56	11.57	0.000 43	3.32	6.11	0.584	1.132	0.0063	0.0086	0.122	0.236	0.003 03	0.052
Nd	60	15.52	0.000 89	4.45	8.11	0.801	1.550	0.0104	0.0139	0.172	0.334	0.0052	0.071
Tb	65	21.75	0.002 13	6.26	11.23	1.148	2.220	0.0182	0.0239	0.252	0.49	0.0094	0.098
Yb	70	29.65	0.0048	8.59	15.13	1.595	3.08	0.0303	0.0388	0.355	0.69	0.0159	0.130
Ta	73	35.3	0.0076	10.27	17.89	1.915	3.70	0.040	0.051	0.43	0.84	0.0216	0.182
W	74	37.4	0.0088	10.88	18.88	2.031	3.92	0.044	0.055	0.46	0.90	0.0239	0.202
Pt	78	46.6	0.0158	13.60	23.24	2.547	4.92	0.062	0.077	0.59	1.16	0.0351	0.293
Au	79	49.1	0.0182	14.36	24.43	2.689	5.20	0.067	0.083	0.63	1.23	0.0386	0.320
Hg	80	51.7	0.0210	15.15	25.66	2.837	5.49	0.073	0.090	0.67	1.31	0.042	0.352
Tl	81	54.4	0.0241	15.97	26.94	2.990	5.79	0.079	0.096	0.71	1.39	0.046	0.385
Pb	82	57.3	0.0277	16.83	28.25	3.15	6.10	0.086	0.104	0.75	1.48	0.050	0.42
Th	90	84.0	0.080	25.00	40.38	4.63	9.03	0.154	0.178	1.15	2.31	0.096	0.80
U	92	91.8	0.103	27.45	43.88	5.07	9.90	0.177	0.202	1.27	2.56	0.112	0.91

TABLE II. Calculated L_{I} x-ray emission rates (eV/$\hbar$).

Element	Z	Total	L_{III} $2p_{3/2}$	M_{II} $3p_{1/2}$	M_{III} $3p_{3/2}$	M_{IV} $3d_{3/2}$	M_{V} $3d_{5/2}$	N_{II} $4p_{1/2}$	N_{III} $4p_{3/2}$	N_{IV} $4d_{3/2}$	N_{V} $4d_{5/2}$	O_{II} $5p_{1/2}$	O_{III} $5p_{3/2}$
Cu	29	0.004 55		0.001 57	0.002 88								
Kr	36	0.0168	0.000 15	0.0054	0.0096			0.000 51	0.000 90				
Rb	37	0.0198	0.000 17	0.0063	0.0112			0.000 71	0.001 25				
Zr	40	0.0314	0.000 24	0.0098	0.0171			0.001 42	0.002 50				
Mo	42	0.0412	0.000 31	0.0129	0.0222			0.002 01	0.003 49				
Ag	47	0.0761	0.000 57	0.0238	0.0396	0.000 26	0.000 39	0.0043	0.0071				
Sn	50	0.1066	0.000 82	0.0331	0.0539	0.000 42	0.000 62	0.0065	0.0107			0.000 15	0.000 23
Sb	51	0.1188	0.000 93	0.0368	0.0594	0.000 49	0.000 72	0.0074	0.0121			0.000 30	0.000 48
Ba	56	0.1988	0.001 72	0.0604	0.0934	0.000 97	0.001 45	0.0136	0.0217			0.002 01	0.0032
Nd	60	0.2830	0.002 83	0.0871	0.1297	0.001 62	0.002 42	0.0202	0.0312	0.000 22	0.000 33	0.0029	0.0044
Tb	65	0.422	0.0053	0.1330	0.1875	0.002 93	0.0044	0.031	0.046	0.000 40	0.000 61	0.0043	0.0061
Yb	70	0.608	0.0097	0.197	0.260	0.0051	0.0076	0.047	0.066	0.000 69	0.001 07	0.0062	0.0082
Ta	73	0.751	0.0141	0.245	0.311	0.0069	0.0104	0.060	0.080	0.000 97	0.001 51	0.0089	0.0116
W	74	0.804	0.0159	0.264	0.330	0.0077	0.0115	0.065	0.086	0.001 08	0.001 69	0.0100	0.0129
Pt	78	1.047	0.0258	0.348	0.408	0.0113	0.0169	0.088	0.110	0.001 67	0.002 62	0.0153	0.0186
Au	79	1.117	0.0292	0.373	0.430	0.0124	0.0186	0.094	0.117	0.001 85	0.002 92	0.0169	0.0203
Hg	80	1.190	0.033	0.398	0.451	0.0137	0.0205	0.101	0.124	0.002 06	0.0032	0.0187	0.0223
Tl	81	1.267	0.037	0.426	0.474	0.0150	0.0225	0.109	0.132	0.002 28	0.0036	0.0207	0.0245
Pb	82	1.349	0.042	0.455	0.496	0.0165	0.0246	0.117	0.139	0.002 53	0.0040	0.0229	0.0268
Th	90	2.181	0.108	0.755	0.690	0.033	0.050	0.202	0.210	0.0056	0.0089	0.048	0.050
U	92	2.441	0.137	0.854	0.739	0.040	0.059	0.231	0.229	0.0068	0.0108	0.056	0.056

TABLE III. Calculated L_{II} x-ray emission rates (eV/$\hbar$).

Element	Z	Total	M_{I} $3s_{1/2}$	M_{III} $3p_{3/2}$	M_{IV} $3d_{3/2}$	N_{I} $4s_{1/2}$	N_{III} $4p_{3/2}$	N_{IV} $4d_{3/2}$	N_{VI} $4f_{5/2}$	O_{I} $5s_{1/2}$	O_{IV} $5d_{3/2}$
Cu	29	0.0055	0.000 30		0.0052						
Kr	36	0.0247	0.000 87		0.0237	0.000 11					
Rb	37	0.0293	0.001 00		0.0281	0.000 14					
Zr	40	0.0472	0.001 47		0.0450	0.000 24		0.000 55			
Mo	42	0.0638	0.001 88		0.0595	0.000 32		0.0020			
Ag	47	0.1253	0.0033		0.1109	0.000 63		0.0104			
Sn	50	0.1786	0.0045		0.1544	0.000 91		0.0186			
Sb	51	0.1996	0.0049		0.1715	0.001 02		0.0221			
Ba	56	0.334	0.0078		0.2790	0.001 77		0.0451		0.000 31	
Nd	60	0.480	0.0109		0.398	0.002 55		0.067		0.000 44	
Tb	65	0.723	0.0161	0.000 39	0.598	0.0039		0.104		0.000 64	

TABLE III. Calculated L_{II} x-ray emission rates ($eV/\hbar$) (*continued*).

Element	Z	Total	M_I $3s_{1/2}$	M_{III} $3p_{3/2}$	M_{IV} $3d_{3/2}$	N_I $4s_{1/2}$	N_{III} $4p_{3/2}$	N_{IV} $4d_{3/2}$	N_{VI} $4f_{5/2}$	O_I $5s_{1/2}$	O_{IV} $5d_{3/2}$
Yb	70	1.051	0.0232	0.000 68	0.866	0.0056		0.154		0.000 90	
Ta	73	1.303	0.0286	0.000 91	1.065	0.0070		0.196	0.000 48	0.001 24	0.0036
W	74	1.397	0.031	0.001 01	1.138	0.0076		0.212	0.000 56	0.001 37	0.0059
Pt	78	1.836	0.040	0.001 47	1.471	0.0100	0.000 39	0.287	0.000 98	0.001 99	0.0229
Au	79	1.962	0.042	0.001 61	1.565	0.0108	0.000 43	0.309	0.001 12	0.002 18	0.0291
Hg	80	2.094	0.045	0.001 76	1.664	0.0115	0.000 48	0.332	0.001 27	0.002 39	0.034
Tl	81	2.233	0.048	0.001 92	1.767	0.0124	0.000 53	0.357	0.001 43	0.002 62	0.041
Pb	82	2.378	0.051	0.002 09	1.875	0.0132	0.000 58	0.383	0.001 61	0.002 86	0.047
Th	90	3.84	0.083	0.0041	2.939	0.0222	0.001 20	0.653	0.0038	0.0056	0.122
U	92	4.29	0.093	0.0047	3.27	0.0251	0.001 43	0.740	0.0046	0.0065	0.143

TABLE IV. Calculated L_{III} x-ray emission rates (eV/$\hbar$).

Element	Z	Total	M_I $3s_{1/2}$	M_{II} $3p_{1/2}$	M_{III} $3p_{3/2}$	M_{IV} $3d_{3/2}$	M_V $3d_{5/2}$	N_I $4s_{1/2}$	N_{IV} $4d_{3/2}$	N_V $4d_{5/2}$	$N_{VI, VII}$ $4f_{5/2, 7/2}$	O_I $5s_{1/2}$	$O_{IV, V}$ $5d_{3/2, 5/2}$
Cu	29	0.0054	0.000 31			0.000 51	0.0046						
Kr	36	0.0241	0.000 96			0.002 33	0.0207	0.000 12					
Rb	37	0.0285	0.001 11			0.002 75	0.0245	0.000 15					
Zr	40	0.0458	0.001 68			0.0044	0.0389	0.000 27	0.000 05	0.000 47			
Mo	42	0.0616	0.002 17			0.0058	0.0513	0.000 37	0.000 20	0.001 73			
Ag	47	0.1196	0.0039			0.0107	0.0946	0.000 75	0.000 98	0.0086			
Sn	50	0.1696	0.0054			0.0147	0.1308	0.001 10	0.001 75	0.0155			
Sb	51	0.1891	0.0061			0.0163	0.1449	0.001 25	0.002 06	0.0183			
Ba	56	0.313	0.0100			0.0263	0.2328	0.002 25	0.0041	0.0368		0.000 39	
Nd	60	0.445	0.0146			0.0371	0.329	0.0033	0.0061	0.054		0.000 58	
Tb	65	0.661	0.0226	0.000 19	0.000 18	0.0550	0.486	0.0053	0.0092	0.082		0.000 88	
Yb	70	0.947	0.034	0.000 33	0.000 30	0.078	0.693	0.0081	0.0132	0.118		0.001 29	
Ta	73	1.163	0.043	0.000 44	0.000 40	0.096	0.843	0.0103	0.0165	0.148	0.000 47	0.001 81	0.0029
W	74	1.244	0.047	0.000 48	0.000 44	0.102	0.898	0.0112	0.0178	0.159	0.000 55	0.002 02	0.0047
Pt	78	1.612	0.063	0.000 70	0.000 63	0.130	1.145	0.0154	0.0235	0.212	0.000 97	0.0030	0.0179
Au	79	1.717	0.068	0.000 76	0.000 69	0.138	1.214	0.0166	0.0251	0.227	0.001 10	0.0033	0.0225
Hg	80	1.826	0.073	0.000 82	0.000 75	0.146	1.285	0.0180	0.0269	0.242	0.001 25	0.0037	0.0267
Tl	81	1.940	0.079	0.000 90	0.000 81	0.154	1.360	0.0194	0.0287	0.259	0.001 41	0.0041	0.032
Pb	82	2.060	0.085	0.000 98	0.000 88	0.163	1.438	0.0209	0.031	0.277	0.001 60	0.0045	0.037
Th	90	3.23	0.147	0.001 84	0.001 67	0.249	2.186	0.037	0.049	0.451	0.0038	0.0092	0.091
U	92	3.59	0.167	0.002 13	0.001 93	0.274	2.410	0.043	0.055	0.506	0.0046	0.0108	0.106

TABLE V. Relative errors in the $E1$ decay rates estimated from the errors in the x-ray and binding energies.

	Transition				
Z	K-L	K-M	K-N	L-M	L-N
37	0.004	0.02	0.06	0.04	0.06
50	0.0011	0.004	0.016	0.012	0.02
80	0.006	0.008	0.017	0.005	0.010

TABLE VI. Total K-shell emission rates of the various multipoles for $_{92}$U.

Multipole	$E1$	$E2$	$E3$	
Rate (eV/$\hbar$)	90.8	0.510	2.78(−4)	
Multipole	$M1$	$M2$	$M3$	$M4$
Rate (eV/$\hbar$)	0.150	0.40	3.1(−3)	1.89(−6)

TABLE VII. Total f values and transition rates for K-N transitions in $_{92}$U.

Level	Multipole	f value	Rate (eV/$\hbar$)
N_{I}	$M1$	2.57(−5)	9.7(−3)
N_{II}	$E1$	3.4(−3)	1.27
N_{III}	$E1$	6.7(−3)	2.54
N_{III}	$M2$	5.7(−5)	2.16(−2)
N_{IV}	$E2$	1.36(−4)	5.2(−2)
N_{IV}	$M1$	1.42(−7)	5.4(−5)
N_{V}	$E2$	1.54(−4)	5.9(−2)
N_{V}	$M3$	1.85(−6)	7.1(−4)
N_{VI}	$E3$	3.5(−7)	1.35(−4)
N_{VI}	$M2$	1.45(−10)	5.5(−8)
N_{VII}	$E3$	3.6(−7)	1.37(−4)
N_{VII}	$M4$	4.8(−9)	1.85(−6)

rates depends on the states being mixtures of different angular momentum components (except in the case of transitions between levels differing at most in the total angular momentum such as the L_{III}-L_{II} transition).[20] The nonvanishing of the L_{I}-K transition in the present calculation is due to retardation and relativistic effects. The values for these rates would be sensitive to corrections bringing in mixtures of angular momentum states.

Parratt[21] gives the radiative decay rates for the K shell based on experimental data for a number of elements, while Callan[22] gives a fit across the periodic table. In Table VIII the present theoretical results based on the Hartree-Slater model are compared with the experimentally deduced values. The agreement is quite satisfactory.

ACKNOWLEDGMENT

The author is indebted to Dr. William Grasberger for bringing to his attention the problem of the relativistic transition rates.

TABLE VIII. Experimental and theoretical total K-shell x-ray emission rates in units of (eV/$\hbar$).

	$_{16}$S	$_{18}$Ar	$_{22}$Ti	$_{25}$Mn	$_{29}$Cu	$_{32}$Ge	$_{36}$Kr	$_{42}$Mo	$_{47}$Ag	$_{79}$Au
Present theory	0.0398	0.0717	0.1860	0.332	0.642	0.996	1.686	3.33	5.42	49.1
Expt. (Parratt[21])	0.04	0.07	0.2	0.33	0.65	1.0	1.7	3.6	6.0	50
Expt. (Callan[22])	0.05	0.09	0.19	0.32	0.59	1.00	2.10	3.89	6.10	49.57

*This work was performed under the auspices of the U. S. Atomic Energy Commission.

[1]H. S. W. Massey and E. H. S. Burhop, Proc. Cambridge Phil. Soc. 32, 461 (1936).

[2]W. Lasker, J. Phys. Radium 16, 644 (1955); Ann. Phys. (Paris) 13, 258 (1958).

[3]W. B. Payne and J. S. Levinger, Phys. Rev. 101, 1020 (1956).

[4]W. N. Asaad, Proc. Roy. Soc. (London) A249, 555 (1959).

[5]G. R. Taylor and W. B. Payne, Phys. Rev. 118, 1549 (1960).

[6]F. A. Babushkin, Acta Physiol. Polon. 25, 749 (1964); Opt. i Spektroskopiya 19, 3 (1965) [English transl.: Opt. Spectry. (USSR) 19, 1 (1965)]; Acta Physiol. Polon. 31, 459 (1967).

[7]See, for example, J. M. Jauch and F. Rohlich, The Theory of Photons and Electrons (Addison-Wesley Publishing Co., Inc., Reading, Mass., 1955), p. 363.

[8]M. E. Rose, Multipole Fields (John Wiley & Sons, Inc., New York, 1955), p. 73.

[9]S. A. Moszkowski, in Alpha-, Beta-, and Gamma-Ray Spectroscopy, edited by K. Siegbahn (North-Holland Publishing Co., Amsterdam, 1965), Chap. XV.

[10]M. E. Rose, G. H. Goestzel, B. I. Spinrad, J. Harr, and P. Strong, Phys. Rev. 83, 79 (1951); and Ref. 8, p. 65 *ff*.

[11]The results are given by Babushkin, Ref. 6.

[12]See, for example, Ref. 8, pp. 92 and 93.
[13]F. Herman and S. Skillman, Atomic Structure Calculations (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963).
[14]D. Liebermann, J. T. Waber, and D. T. Cromer, Phys. Rev. 137, A27 (1965); see also C. W. Nestor *et al.*, Oak Ridge National Laboratory Report No. ORNL-4027, 1966 (unpublished), and T. A. Carlson *et al.*, Phys. Rev. 169, 27 (1968).
[15]L. S. Foster, in Handbook of Chemistry and Physics, edited by Robert C. Weast (The Chemical Rubber Co., Cleveland, Ohio, 1966), p. B-2.
[16]S. T. Manson and J. W. Cooper, Phys. Rev. 165, 126 (1968).
[17]J. A. Bearden, Rev. Mod. Phys. 39, 78 (1967); J. A. Bearden and A. F. Burr, *ibid.* 39, 125 (1967).
[18]See J. C. Slater, Phys. Rev. 98, 1039 (1955).
[19]A calculation of the effect of the finite nuclear size on the transition rates is given by F. A. Babushkin, Zh. Eksperim. i Teor. Fiz. 48, 561 (1965) [English transl.: Soviet Phys. – JETP 21, 372 (1965)]. Results for the various corrections of the binding energy are given by D. F. Mayers, G. E. Brown, and E. A. Sanderson, Phys. Rev. Letters 3, 90 (1959). Relativistic calculations with the more complete Hartree-Fock model are given by Y. K. Kim, Phys. Rev. 154, 17 (1967); M. A. Coulthard, Proc. Phys. Soc. (London) 91, 44 (1967); and F. C. Smith and W. R. Johnson, Phys. Rev. 160, 136 (1967). For a summary of the corrections see Ref. 20, Chaps. I and II.
[20]See H. A. Bethe and E. E. Salpeter, Quantum Mechanics of One- and Two-Electron Atoms (Springer-Verlag, Berlin, 1957), p. 282 *ff.*
[21]L. G. Parratt, Rev. Mod. Phys. 31, 616 (1959).
[22]E. J. Callan, in Proceedings of the Conference on Atomic Electrons in Nuclear Transformations (Nuclear Energy Information Center, Warsaw, Poland, 1963), Vol. III, p. 419.

PHYSICAL REVIEW VOLUME 179, NUMBER 1 5 MARCH 1969

Difficulties of the Independent-Particle Model in the Description of Energetic Transitions in Atoms

S. Hameed*

Theoretical Physics Department, University of Manchester, England

(Received 19 August 1968)

It is shown that the first-order correlation correction to the transition matrix element between two nonpenetrating states can be written in a completely parametrized form. The correction is directly proportional to the square of the transition energy and to the dipole polarizability of the core. It follows that for sufficiently energetic transitions the magnitude of the correction becomes as large as the zero-order matrix element.

INTRODUCTION

Hartree-Fock transition probabilities deviate significantly from experimental values. Recently first-order correlation corrections to the lowest $s \rightarrow p$ oscillator strengths have been calculated for alkali atoms,[1,2] and they are found to be essential in order to have agreement between theory and experiment. In the independent-particle picture, optical transitions in an alkali atom occur by the excitation of the single valence electron. The valence electron is very loosely bound compared to the core electrons. This fact simplifies the treatment of correlation effects because the valence and core charge distributions overlap very little. One consequence of this is that exchange between the valence electron and the core electrons plays a minor role.

Here we study states with high angular momenta in which the probability density of the valence electron in the region of the core is almost zero. These are referred to as "nonpenetrating" states and their properties differ from the corresponding hydrogen properties mainly because of correlation effects. To illustrate, the Hartree-Fock (H.F.) eigenvalue (calculated by the Herman-Skillman method) of the single-particle $4f$ level of potassium is $-0.031\,27$ a.u., the corresponding hydrogen eigenvalue being $-0.031\,25$ a.u. The empirical value is $-0.031\,34$ a.u. (atomic units are used in this paper). The H.F. $4f$ wave function of potassium $P_{4f}(r)$, with normalization

$$\int_0^\infty [P_{4f}(r)]^2 dr = 1,$$

is shown in Fig. 1. The corresponding hydrogen