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K-MM Auger-intensity peaks from double-hole energy-level crossings

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Relativistic computations of *K-MM* Auger spectra have been carried out in the intermediate-coupling scheme with configuration interaction. Good agreement with the scarce experimental data is attained. The calculated K-$M_1M_{4,5}$ intensity is found to peak sharply in the neighborhood of $Z=63$. This peculiar behavior is traced to the crossings of two-*M*-hole energy levels, as functions of atomic number.

I. INTRODUCTION

The effects of relativity, spin-orbit mixing, and configuration interaction have been found to be very important in analyzing the *K-LL* Auger spectrum.[1,2] Recently, the relativisitc *K-MM* relative intensity in j-j coupling and the relative intensity from nonrelativistic intermediate coupling have been found to disagree with experimental values for medium-Z and heavy elements.[3,4] To resolve this discrepancy, we have extended the same technique previously used in the analysis of *K-LL* Auger spectra[1,2] to treat the *K-MM* Auger spectra of medium-Z and heavy elements.

In this paper we report on the theoretical *K-MM* Auger spectra from Dirac-Hartree-Slater (DHS) calculations in intermediate coupling with final-hole-state configuration interaction, for 10 elements with $36 \leq Z \leq 92$. The effect of channel coupling, neglected in the present calculations, could be important for light atoms.[5] Elements with $Z < 36$ are therefore not included in our present work.

II. THEORY

From perturbation theory, in the frozen-orbital approximation, the Auger transition probability in j-j coupling is

$$T(\alpha JM \rightarrow \alpha' J'M') = |\langle j_1' j_2' J'M' | V_{12} | j_1 j_2 JM \rangle|^2 \ . \quad (1)$$

Here, $|j_1' j_2' J'M'\rangle$ represents the initial two-hole coupled state including the initial bound-state hole j_1' and the hole j_2' in the continuum that is filled by the emitted Auger electron. The final two-hole-coupled state is denoted by $|j_1 j_2 JM\rangle$. The continuum wave function is normalized so as to represent one electron ejected per unit time. Atomic units are used unless indicated otherwise. Coupling between an outermost open shell and inner-shell vacancies is neglected in Eq. (1). No appreciable Auger-electron energy shift is introduced by such coupling in transitions discussed in this paper, whence the rates are independent of the passive electron structure.[6] The two-electron operator V_{12} is chosen according to the original Møller formula[7] which is in the Lorentz gauge,

$$V_{12} = (1 - \vec{\alpha}_1 \cdot \vec{\alpha}_2) \exp(i\omega r_{12})/r_{12} \ ,$$

where the $\vec{\alpha}_i$ are Dirac matrices, and ω is the wave number of the virtual photon.

Configuration interaction among all the possible final-double-*MM*-hole states is included in the calculations. For these calculations, j-j coupled basis states are used. In a j-j basis set, intermediate coupling can be treated as configuration interaction. Coulomb as well as Breit interactions are included in the energy matrix. The eigenfunctions and eigenvalues are obtained by diagonalizing the energy matrix. For example, for a $J=0$ state, the interactions among $M_1M_1(J=0)$, $M_2M_2(J=0)$, $M_3M_3(J=0)$, $M_4M_4(J=0)$, and $M_5M_5(J=0)$ are included in our present calculations. The detailed treatment of relativistic intermediate coupling with configuration interaction is described in Ref. 1.

The relativistic Auger matrix elements in j-j coupling were calculated from DHS wave functions that correspond to the initial-hole-state configuration.[8] In the configuration-interaction calculations, the j-j configuration average energies were calculated from DHS wave functions[9] with the appropriate final-hole-state configurations including quantum-electrodynamic corrections. The energy splittings of the specific total J states of the two-hole-coupled configurations and off-diagonal matrix elements of the energy matrix were calculated by using a slightly modified general Auger program[8] which includes Coulomb and Breit interactions. Eigenvalues and eigenfunctions were obtained by diagonalizing the energy matrix. The eigenfunctions obtained in diagonalizing the energy matrix were then incorporated in relativistic matrix elements to calculate the transition rates.

III. RESULTS AND DISCUSSION

The calculated relativistic *K-MM* Auger transition rates in intermediate coupling with configuration interaction are listed in Table I. Our present DHS *j-j* coupling results agree with those of other relativistic calculations.[10,11] The relative intensities of the K-M_1M_1, K-M_1M_2, K-M_2M_2, K-M_2M_3, K-$M_2M_{4,5}$, and K-$M_3M_{4,5}$ transitions with respect to the sum of *K-MM* transition rates (excluding K-$M_{4,5}M_{4,5}$) from Dirac-Hartree-Slater and Hartree-Slater calculations and experiment are compared in Figs. 1 and 2. The relativistic effects are quite large on most of the *K-MM* transitions (e.g., approximately a factor of 2 at $Z=80$ for K-M_1M_1). Intermediate coupling and configuration interaction drastically improve the agreement between the theoretical and experimental K-M_iM_j intensity ratios. The effects of configuration interaction among $M_1M_1(J=0)$, $M_2M_2(J=0)$, and $M_3M_3(J=0)$ states persist to the heavy elements, similar to the case of $L_1L_1(J=0)$, $L_2L_2(J=0)$, and $L_3L_3(J=0)$.[1,2] Very good agreement between theory and experiment[3,4,12] is attained for K-M_1M_1, K-M_1M_2, and K-M_2M_3 transitions after including configuration interaction. For K-$M_2M_{4,5}$ and K-$M_3M_{4,5}$ transitions, fair agreement is found between theory and experiment, considering the scarcity of experimental data.

The K-$M_1M_{4,5}$ intensity has a strong peak at $Z\approx 63$ (Fig. 3). This peculiar behavior is caused by level crossing. For $Z<60$, the $M_3M_3(J=2)$ level lies above the $M_1M_4(J=2)$ and $M_1M_5(J=2)$ levels. As Z increases, $M_3M_3(J=2)$ first comes down to cross $M_1M_4(J=2)$ at $Z\approx 62$, then crosses $M_1M_5(J=2)$ at $Z\approx 65$ (Fig. 4). The K-$M_1M_{4,5}$ transitions pick up some intensity from K-M_3M_3

TABLE I. Theoretical relativistic *K-MM* Auger transition rates (in milliatomic units[a]), in intermediate coupling with configuration interaction.[b]

Final state \ Z	36	45	54	60	65	67	70	92
M_1M_1	4.30(−2)	6.93(−2)	1.05(−1)	1.36(−1)	1.68(−1)	1.82(−1)	2.06(−1)	5.05(−1)
M_1M_2	1.01(−1)	1.34(−1)	1.63(−1)	1.98(−1)	2.41(−1)	2.62(−1)	3.00(−1)	9.21(−1)
M_1M_3	3.13(−2)	6.53(−2)	1.19(−1)	1.54(−1)	1.83(−1)	1.95(−1)	2.12(−1)	3.49(−1)
M_2M_2	2.40(−2)	2.54(−2)	2.70(−2)	2.89(−2)	3.07(−2)	3.15(−2)	3.28(−2)	4.40(−2)
M_2M_3	2.21(−1)	2.86(−1)	3.33(−1)	3.63(−1)	3.88(−1)	3.98(−1)	4.14(−1)	5.20(−1)
M_3M_3	2.24(−2)	6.50(−2)	1.05(−1)	9.20(−2)	1.15(−1)	1.57(−1)	1.94(−1)	2.73(−1)
M_1M_4	1.66(−2)	2.18(−2)	3.03(−2)	6.34(−2)	1.31(−2)	1.08(−2)	1.31(−2)	3.55(−2)
M_1M_5	6.30(−3)	1.20(−2)	1.87(−2)	3.18(−2)	8.45(−2)	5.41(−2)	2.81(−2)	2.21(−2)
M_2M_4	1.68(−3)	1.64(−3)	1.09(−2)	1.37(−2)	1.60(−2)	1.70(−2)	1.86(−2)	3.35(−2)
M_2M_5	3.43(−2)	5.52(−2)	5.33(−2)	5.62(−2)	5.71(−2)	5.77(−2)	5.84(−2)	6.10(−2)
M_3M_4	5.37(−3)	1.59(−2)	3.56(−2)	4.64(−2)	5.29(−2)	5.53(−2)	5.84(−2)	7.22(−2)
M_3M_5	1.63(−2)	2.45(−2)	2.84(−2)	3.43(−2)	3.97(−2)	4.17(−2)	4.46(−2)	6.07(−2)
M_4M_4	1.30(−4)	1.66(−4)	1.10(−4)	8.72(−5)	7.08(−5)	7.07(−5)	6.62(−5)	1.11(−4)
M_4M_5	8.68(−5)	4.37(−3)	5.40(−3)	6.74(−3)	7.27(−3)	7.95(−3)	7.89(−3)	9.04(−3)
M_5M_5	4.33(−4)	9.21(−4)	1.36(−3)	7.09(−4)	9.14(−4)	1.04(−3)	1.10(−3)	1.81(−3)

[a] 1×10^{-3} a.u. $=0.027\,21$ eV/$\hbar=4.134\times10^{13}$ s^{-1}.

[b] Numbers in parentheses signify powers of ten, e.g., $4.30(-2)=4.30\times10^{-2}$.

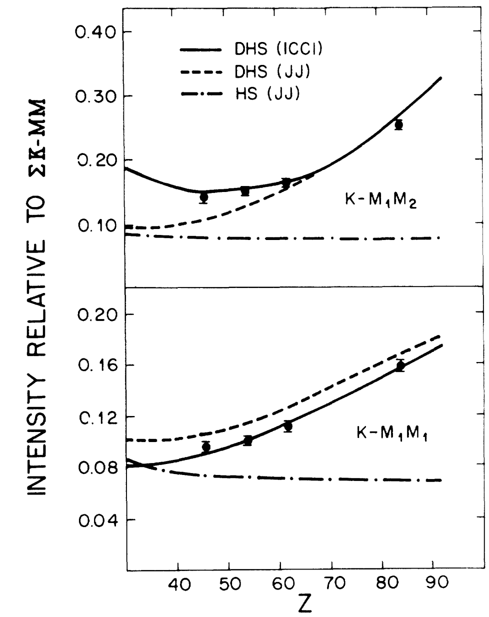

FIG. 1 Ratio of calculated K-M_1M_2 and K-M_1M_1 Auger-transition rates to the total K-MM transition rate (excluding K-$M_3M_{4,5}$), as a function of atomic number. The solid curve represents Dirac-Hartree-Slater results in intermediate coupling with configuration interaction, the dashed curves indicate Dirac-Hartree-Slater results in j-j coupling, and the dot-dashed curves represent nonrelativistic Hartree-Slater results in j-j coupling, all from the present work. The experimental results are from Refs. 3, 4, and 12.

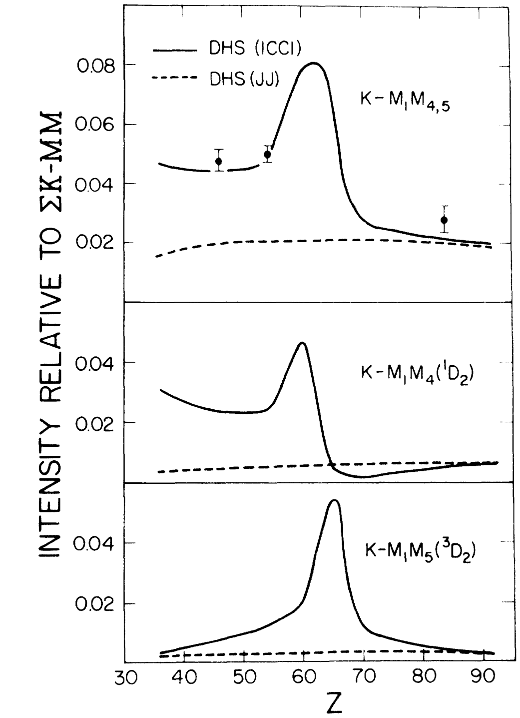

FIG. 3. Ratio fo K-$M_1M_{4,5}$ Auger-transition rates to the total K-MM rate, as functions of atomic number. The Dirac-Hartree-Slater calculation in intermediate coupling with configuration interaction (solid curves) exhibits a pronounced peak near $Z=63$, caused by level crossing (see text). The broken curves represent Dirac-Hartree-Slater results in j-j coupling. Experimental data are from Refs. 3, 4, and 12.

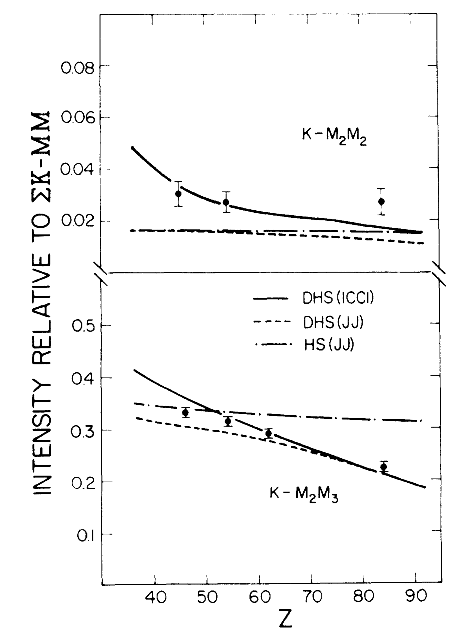

FIG. 2. Ratio of calculated K-M_2M_2 and K-M_2M_3 Auger-transition rates to the total K-MM rate; see caption of Fig. 1 for details.

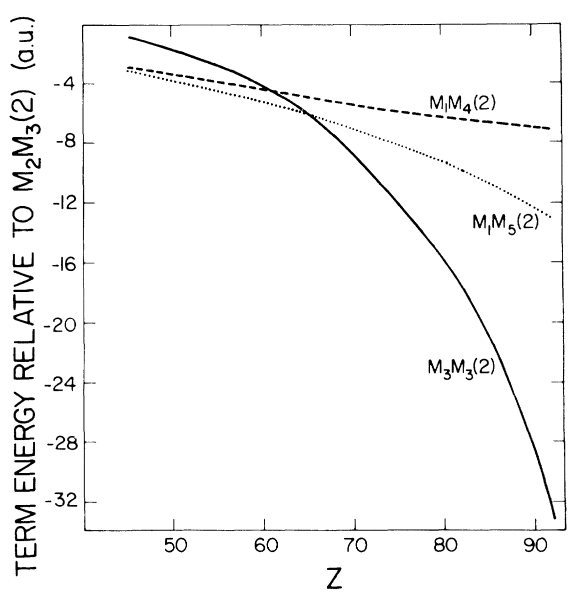

FIG. 4. Two-hole M-shell energy levels, as functions of atomic number. Level crossings cause the Auger-intensity peaks illustrated in Fig. 3.

through the strong configuration interaction between $M_1M_{4,5}(J=2)$ and $M_3M_3(J=2)$ states. The K-$M_1M_{4,5}$ transition rate increases by a factor of ~ 4 at $Z \approx 63$ and by a factor of ~ 2 for $Z < 55$. Good agreement between theory and experiment is obtained for K-$L_1M_{4,5}$ intensity ratios after including level-crossing interaction (cf. Fig. 3). Level crossing is a very common phenomenon in multiply ionized atoms.[13] Great care has to be taken in treating these cases.

[1]M. H. Chen, B. Crasemann, and H. Mark, Phys. Rev. A 21, 442 (1980).
[2]W. N. Asaad and D. Petrini, Proc. R. Soc. London, Ser. A 350, 381 (1976).
[3]M. I. Babenkov, B. V. Bobykin, V. S. Zhdanov, and V. K. Petukhov, J. Phys. B 15, 35 (1982).
[4]M. I. Babenkov, B. V. Bobykin, V. S. Zhdanov, and V. K. Petukhov, J. Phys. B 15, 927 (1982).
[5]G. Howat, T. Åberg, and O. Goscinski, J. Phys. B 11, 1575 (1978).
[6]E. J. McGuire, in *Atomic Inner-Shell Processes,* edited by B. Crasemann (Academic, New York, 1975), Vol. I, p. 293.
[7]C. Møller, Ann. Phys. (Leipzig) 14, 531 (1932).
[8]M. H. Chen, E. Laiman, B. Crasemann, M. Aoyagi, and H. Mark, Phys. Rev. A 19, 2253 (1979).
[9]K. N. Huang, M. Aoyagi, M. H. Chen, B. Crasemann, and H. Mark, At. Data Nucl. Data Tables 18, 243 (1976).
[10]C. P. Bhalla and D. J. Ramsdale, Z. Phys. 239, 95 (1970).
[11]C. P. Bhalla, H. R. Rosner, and D. J. Ramsdale, J. Phys. B 3, 1232 (1970).
[12]M. I. Babenkov, B. V. Bobykin, V. S. Zhdanov, and V. K. Petukhov, Phys. Lett. 56A, 363 (1976).
[13]A. W. Weiss, in *Beam-Foil Spectroscopy,* edited by I. A. Sellin and D. J. Pegg (Plenum, New York, 1976).