At $T=300°K$, Eq. (20) gives

$$\Delta K_e \sim 5\times 10^{10} \text{ dyne cm}^{-2}, \quad (21)$$

which is again of the required order of magnitude.

(c) Debye Temperature of Palladium

Using the method of DeLaunay[17] to compute θ_0 and taking $\rho_0=12.132$ gram cc^{-3}, $V_0=8.7949$ cm^3, we obtain from the elastic data extrapolated to absolute zero

$$\theta=275-0.06T^2 \text{ °K}. \quad (22)$$

The value $\theta_0=275\pm 8°K$ is in excellent agreement with that obtained by Hoare and Yates,[5] who found from their calorimetric data a value $\theta_0=274\pm 3°K$. Owing to the large electronic heat capacity of palladium, it is difficult to determine the Debye temperature with much accuracy from calorimetry. Their error estimate is a measure only of the internal consistency of the data and hence the above agreement is somewhat misleading, since a small systematic error could easily cause a fairly large change in the calorimetric value of θ. It is believed that an error of this sort is responsible for the higher Debye temperature $\theta_0=299°K$ reported by Rayne.[6] Owing to the small specimen mass used in the latter work, an error in the specific heat of the addenda could easily be responsible for the discrepancy.

It is of interest that measurements in the liquid hydrogen range[18,19] give $\theta=275°K$. This circumstance is difficult to understand since, according to Eq. (22), θ should be considerably lower than the liquid helium value and should be varying quite rapidly with temperature. One possible explanation is that the electronic heat capacity is not constant up to these temperatures, but this hardly seems likely since the degeneracy temperature of the holes in the d band is in excess of 1000°K. It would thus seem desirable to have more accurate heat capacity data in the liquid hydrogen region to check the validity of Eq. (22).

[17] J. DeLaunay, in *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1956), Vol. 2, p. 285.

V. CONCLUSION

Elastic data have been obtained on a single crystal of palladium from 4.2–300°K. The data extrapolated to absolute zero give a value of Debye temperature in good agreement with that obtained from calorimetry. The anomalous behavior of C and C' is satisfactorily correlated with the temperature dependence of the contribution to the shear constants, arising from the holes in the d band of palladium.

ACKNOWLEDGMENT

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[18] G. L. Pickard and F. Simon, Proc. Phys. Soc. (London) **61**, 1 (1948).
[19] K. Clusius and L. Schachinger, Z. Naturforsch. **2a**, 90 (1947)

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Retardation and K X-Ray Relative Intensities*

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The matrix elements for electric dipole transitions with retardation have been numerically evaluated for transitions between the $1s$ and higher discrete states of a single Dirac electron in a Coulomb field. The results are used to calculate the relative intensities of the principal K x-ray lines in elements of high atomic number. Comparison of the retarded and nonretarded matrix elements confirms the earlier result for lead that the effect of retardation is significant in heavy elements only when the total angular momentum of the electron changes. Comparison with the experiments of Beckman indicate that this conclusion is correct, and that in the $K\alpha_2$ to $K\alpha_1$ intensity ratio the effect of retardation is more significant than screening effects.

INTRODUCTION

THE matrix elements for K x-ray transitions in the Dirac hydrogenic atom have been numerically evaluated for atomic numbers ranging from 1 to 100. These matrix elements are presented in algebraic form in an earlier paper[1] and will not be repeated here. The matrix elements have been used to compute the relative intensity (intensity in energy/unit time) of K x-ray lines in heavy elements. These relative intensities are compared first with earlier calculations[2] of these relative intensities in which retardation effects were neglected and with recent experiments.[3]

The intensity of an x-ray transition from an initial state a to a final state b is given in ergs/sec by

$$I_{ab}=(2e^2\hbar/mc^3)\omega_{ab}{}^3 f_{ab}, \quad (1)$$

* Supported by the Research Corporation.
[1] W. B. Payne and J. S. Levinger, Phys. Rev. **101**, 1020 (1956). This paper is referred to throughout this article as (PL).
[2] W. B. Payne, dissertation, Louisiana State University, 1955 (unpublished).
[3] O. Beckman, Arkiv Fysik **9**, 495 (1955).

TABLE I. K x-ray intensities (ergs/sec).

Z	$K\alpha_2$	$K\alpha_1$	$K\beta_3$	$K\beta_1$	$K\beta_2'$	$K\beta_2''$
29 rel	6.15×10^{6}	1.25×10^{7}	1.87×10^{6}	3.87×10^{6}	8.18×10^{5}	1.70×10^{6}
ret	6.12×10^{6}	1.22×10^{7}	1.92×10^{6}	3.89×10^{6}	8.20×10^{5}	1.67×10^{6}
47 rel	1.13×10^{8}	2.36×10^{8}	3.40×10^{7}	7.55×10^{7}	1.44×10^{7}	3.25×10^{7}
ret	1.13×10^{8}	2.23×10^{8}	3.45×10^{7}	7.17×10^{7}	1.46×10^{7}	3.09×10^{7}
56 rel	3.28×10^{8}	6.91×10^{8}	9.70×10^{7}	2.22×10^{8}	4.08×10^{7}	9.57×10^{7}
ret	3.25×10^{8}	6.41×10^{8}	9.86×10^{7}	2.09×10^{8}	4.14×10^{7}	8.97×10^{7}
82 rel	3.36×10^{9}	7.63×10^{9}	8.94×10^{8}	2.50×10^{9}	3.59×10^{8}	1.08×10^{9}
ret	3.34×10^{9}	6.64×10^{9}	9.49×10^{8}	2.15×10^{9}	3.86×10^{8}	9.37×10^{8}
100 rel	1.13×10^{10}	2.83×10^{10}	2.67×10^{9}	9.47×10^{9}	1.01×10^{9}	4.10×10^{9}
ret	1.15×10^{10}	2.15×10^{10}	2.99×10^{9}	7.43×10^{9}	1.17×10^{8}	3.25×10^{9}

where ω_{ab} is the angular frequency of the emitted x ray and f_{ab} is the oscillator strength.

This paper restricts itself to K x-ray transitions and state b is always the $1s_{\frac{1}{2}}$ state. For these transitions f_{ab} is given in terms of the Dirac radial wave functions in (PL). The oscillator strength neglecting retardation $(f_{ab})_{\text{rel}}$ is given by Eqs. (1) and (2) of (PL); with inclusion of the effect of retardation $(f_{ab})_{\text{ret}}$ is given by Eqs. (3) and (4) of the same paper. Algebraic expressions for these matrix elements for transitions from the second, third, and fourth atomic shells are also given there. These algebraic expressions have been evaluated numerically using an IBM 650 digital computer. The evaluation for all atomic numbers is not presented in this paper, but will be supplied on request to the authors.

No efforts have been made to include effects due to the screening of outer electrons on the overlap integral involved in the matrix elements. The intensity of a given line is proportional to the product of the square of the transition energy and the square of this overlap integral. It is known from numerical calculations[4] with nonrelativistic Coulomb wave functions that use of approximate screening corrections such as the Slater screening constants[5] does not result in a better estimate of these overlap integrals.

On the other hand, using the experimental energy of the x-ray transition instead of that predicted by the Dirac equation in the energy-squared factor of the transition probability can be expected to lead to a better prediction of relative intensity. This substitution will be shown to result in a small but consistent improvement in the agreement between the theoretical curve and the experimental points. Curves in which this substitution has been made are referred to as "retarded, experimental energies."

So far as screening corrections are concerned, one might expect the following to be true in general. First, screening would be least significant for the innermost electrons. Therefore, better agreement between prediction and experiment would be expected for the $K\alpha$ transitions than for transitions which originate in higher atomic shells. It can also be anticipated that screening would have a smaller effect on the relative intensity of doublets than of transitions from different shells.

Second, for the heaviest elements ($Z>70$; which is the range of Beckman's experiments) the difference between one element and the next is the addition of an electron to an outer shell. Therefore, while the inner electrons will have an effect on the magnitude of the relative intensity, the derivative of relative intensity with respect to the atomic number should be less sensitive to screening corrections.

No corrections have been made for the finite size of the nucleus.

RESULTS

For several elements and for each transition considered, Table I gives the intensity in ergs/sec of the x rays. The table shows for comparison the predictions including the effects of retardation, but without the use of experimental x-ray energies, and the calculations using relativistic matrix elements, ignoring retardation. The matrix element involves a small difference between large terms, and the results are probably not more certain than about one percent. In every case for the heavier elements the effect of retardation is a significant reduction in the intensity of transitions in which the total angular momentum changes, and a very much smaller effect for transitions with no change in this quantity.

The calculated intensities have been used to compute

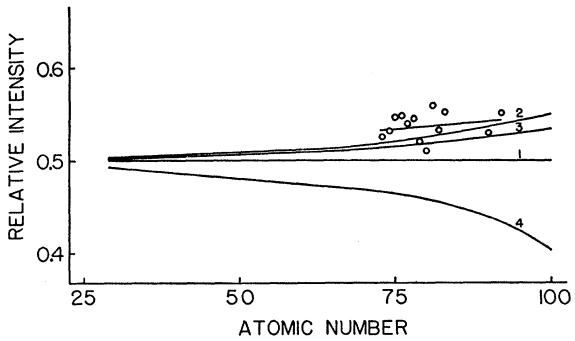

FIG. 1. Relative intensity of $K\alpha_2$ to $K\alpha_1$. In all figures curves are marked (1) nonrelativistic; (2) retarded, experimental energies; (3) retarded, theoretical energies; (4) relativistic, no retardation. The points are Beckman's experimental measurements.

[4] T. F. Tuan, thesis, Louisiana State University, 1953 (unpublished).

[5] J. C. Slater, Phys. Rev. 36, 57 (1930).

the relative intensities of some of the K x-ray lines, and these are shown in the figures. In each figure the curves are marked as follows: Curve 1 shows the predicted relative intensity in the nonrelativistic hydrogenic atom[6]; curve 2 the relativistic calculations with retardation and with the experimental x-ray energies[7] used; curve 3 the relativistic retarded calculations with theoretical x-ray energies; curve 4 the relativistic calculation without retardation and with theoretical energies. Each figure also contains Beckman's experimental points and a least squares fit to these points. Figure 1 shows the intensity ratio $K\alpha_2$ to $K\alpha_1$; Fig. 2 the ratio $K\beta_3$ to $K\beta_1$; Fig. 3 shows $K\beta_1$ to $K\alpha_1$ and Fig. 4 $K\beta_2$ to $K\alpha_1$. In this case $K\beta_2$ refers to the sum of the intensities of the transitions from the $4p$ subshell, since these were not measured separately in Beckman's experiment.

From Figs. 1 and 2, which compare the intensity of transitions from the same atomic subshell, one sees that including retardation improves the agreement with experiment both in absolute value and in slope. In fact, in the case of the $K\alpha$ transitions, the slope of the curve changes sign when retardation is included. Also, it may be seen that use of experimental transition energies results in still better agreement between theory and experiment.

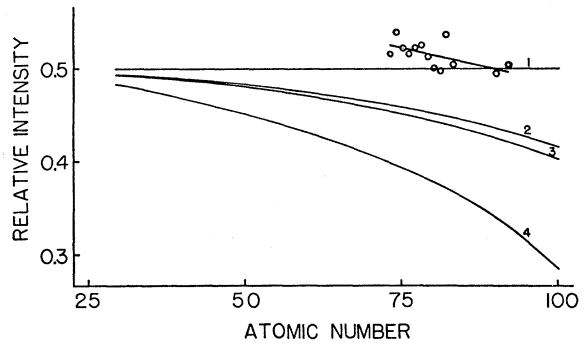

FIG. 2. Relative intensity $K\beta_3$ to $K\beta_1$.

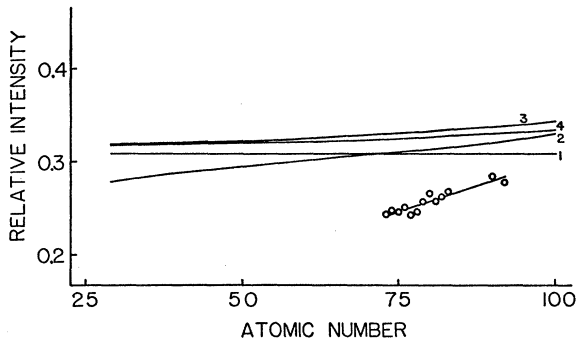

FIG. 3. Relative intensity $K\beta_1$ to $K\alpha_1$.

[6] H. A. Bethe, *Handbuch der Physik*, edited by S. Flügge (Verlag Julius Springer, Berlin, 1933), Vol. XXIV, Part 1, Chap. 3.

[7] R. D. Hill, E. L. Church, and J. W. Mihelich, Rev. Sci. Instr. **23**, 523 (1952).

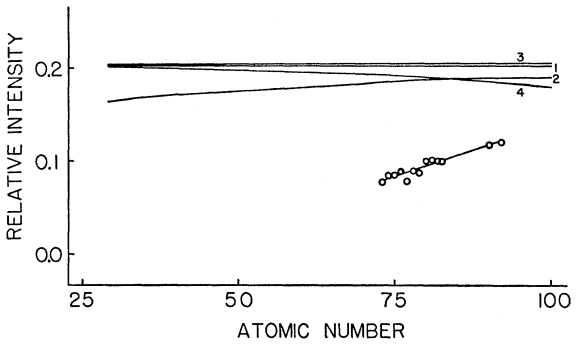

FIG. 4. Relative intensity $K\beta_2$ to $K\alpha_1$.

TABLE II. Average slope of relative intensity curves.

Intensity ratios	Experimental	Retarded[a] (theoretical energies)	Nonretarded[a]
$K\alpha_2/K\alpha_1$	6.23×10^{-4}	6.59×10^{-4}	-6.14×10^{-4}
$K\beta_3/K\beta_1$	-1.43×10^{-3}	-1.72×10^{-3}	-3.52×10^{-3}
$K\beta_1/K\alpha_1$	2.21×10^{-3}	6.16×10^{-4}	2.95×10^{-4}
$K\beta_2/K\alpha_1$	2.23×10^{-3}	1.96×10^{-4}	-3.84×10^{-4}

[a] Average slope from $Z=73$ to 92.

The agreement between the retarded, experimental energy curve and Beckman's experimental points for $K\alpha$ transitions shows that screening could have remarkably little effect on the relative intensity of these transitions. The numerical calculation of this ratio for gold by Massey and Burhop[8] resulted in a value of 0.48. In their calculation relativistic screened wave functions were used, but retardation was ignored. The relativistic calculation with retardation and without screening yields a value of 0.518 for this ratio. The application of screening correction to the retarded calculations of this paper should result in still better agreement with the experiments.

As expected, the agreement between theory and experiment becomes progressively worse when higher atomic states are involved. In every case considered, the slope of the retarded curve is much closer to that of the experimental points than is that of the relativistic curve. Again in the case of the $K\beta_2$ to $K\alpha_1$ ratio the sign of the derivative is changed by including retardation.

Table II gives the slope of the relative intensity curves as determined from a least squares fit to Beckman's data, the average slope over the same range of atomic number of the retarded, theoretical energy curves, and of the relativistic curve without retardation. In every case the inclusion of retardation brings the slope of the curve nearer that of the experiment. In spite of our failure to include screening and other corrections, it is believed that Beckman's experiments provide verification of the prediction of the effects of retardation on relativistic radiative transitions.

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