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Elastic scattering of 88.03-keV γ rays

G. Basavaraju, P. P. Kane, and Saharsha M. Lad Department of Physics, Indian Institute of Technology, Powai, Bombay 400076, India

Lynn Kissel

Computational Physics Group, L-Division, Lawrence Livermore National Laboratory, Livermore, California 94551

R. H. Pratt

Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260 (Received 16 August 1994)

Significant deviations previously reported [Phys. Rev. A 36, 5626 (1987)] between experimental and theoretical cross sections for elastic scattering of 88.03-keV γ rays through 125° have been removed. The present paper shows that the S-matrix treatment is successful in predicting γ -ray elastic-scattering cross sections even very close to K-shell thresholds of high-Z elements.

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I. INTRODUCTION

Differential cross sections for 125° elastic scattering of 88.03-keV γ rays of a ¹⁰⁹Cd source were reported a few years ago [1] in the cases of aluminum, gold, lead, and bismuth. Whereas the measured cross sections in the case of Al and Au were found to be respectively in fair and good agreement with realistic second-order S-matrix calculations, the experimental values for Pb and Bi were larger than the calculated ones by about 3.3 and 4.5 times the stated experimental errors, respectively. Several issues concerning the determination of experimental and theoretical values of these cross sections and of the associated errors are now better understood. As a result, there is now agreement between experiment and theory. Details underlying the changes in theoretical and experimental values are described in Secs. II and III respectively. The conclusions, including a summary presentation of previous and present values in Table I, are stated in Sec. IV.

II. THEORETICAL CALCULATIONS OF CROSS SECTIONS

In the independent-particle approximation, the relativistic second-order S-matrix amplitude for photon scattering is obtained separately for each atomic electron and is summed to give the atomic Rayleigh amplitude. In each electron contribution, there is a sum over a complete set of intermediate states (bound and continuum) of the single-particle Hamiltonian, whether or not such states correspond to occupied orbitals of the atomic system. As pointed out in Ref. [2], transitions to intermediate bound states correspond to resonances in the individual electron amplitude. The resonant transition from a bound state a to an intermediate bound state b corresponding to a filled orbital is canceled by the resonance in the amplitude for scattering from an electron in state b involving a transition to the intermediate state a. These canceling resonances are called spurious resonances. Below a resonance region, the scattering amplitude from that electron is small, and in the low-energy limit it is proportional to the square of the photon energy. Above the photoionization threshold for a given electron, the amplitude for scattering from the electron is close to r_0 in the forward direction, but generally becomes small for scattering vectors [=(momentum transfer)/ħ)] that are large compared to the inverse of the radius of the orbital. Here $r_0 = e^2/(mc^2)$, e is the electron charge, m is the mass of an electron, c is the speed of light, and $\hbar = h/2\pi$ is Planck's constant. However, the amplitude is not small in the vicinity of a real or a spurious resonance.

The scattering amplitude at a given finite angle due to weakly bound outer electrons generally drops rapidly with increasing photon energy $h\nu$. Thus an approximate estimate of outer-electron contributions, such as that provided by the relativistic modified form-factor (MF) approximation, is adequate, whereas an accurate S-matrix calculation is needed in the case of inner shells. Such a procedure was employed in most of the earlier calculations including the ones reported in Refs. [1-3].

However, the MF approximation omits spurious resonances and hence fails to provide the proper cancellation with the spurious resonances of the S-matrix calculation for the inner shells. The errors introduced in this way become particularly serious when the photon energy is close to an inner-shell threshold. Under these circumstances, it is better to first subtract the spurious resonances in the inner-shell contributions so that, shell by shell, the amplitude is finite except for real observable resonances at transitions into unfilled shells. A known analytic form [2] can be used for the bound-bound resonance terms in each

TABLE I. Differential cross sections for the elastic scattering of 88.03-keV γ rays through 125° in 10^{-24} cm²/sr. Cross sections reported in Ref. [1] are indicated as 1987 values. The present values reflect the changes discussed in Secs. II and III.

Element	Calculated cross section		Experimental cross section	
	(1987 value)	(Present value)	(1987 value)	(Present value)
Al	0.001 33	0.001 39	0.0016±0.0002	0.0016±0.0002
Au	0.680	0.666	0.711 ± 0.049	0.711 ± 0.049
Pb	0.424	0.541	$0.604{\pm}0.054$	0.602 ± 0.091
Bi	0.132	0.144	$0.221 {\pm} 0.020$	0.172 ± 0.017

amplitude. Further, as described in Ref. [3], near an inner-shell threshold it is necessary to adopt a photon-energy shifting procedure so that the anomalous scattering region with a rapidly varying amplitude is properly positioned. Note also that a choice of the Dirac-Slater (DS) form instead of the Kohn-Sham (KS) form for the local exchange potential in the electron Hamiltonian can lead to changes in calculated cross sections of the order of 4 and 1% in the cases of low and high Z, respectively.

As in our recent work [3], the subshells with binding energies larger than $h\nu/300$ were considered as inner and treated by S-matrix methods, but now subtracting off the spurious resonances. As before, the MF approximation was used for outer shells. This procedure is efficient in terms of computation time and is also reliable [4].

Binding energies of atomic subshells were obtained from Refs. [5,6]. Data concerning properties of the $^{109}\mathrm{Cd}$ source are available from Refs. [7,8]. In view of small, but noticeable differences between the different compilations, a value of 27 ± 7 eV was adopted for the excess of photon energy $h\nu$ over the lead K-shell binding energy ϵ_K . The calculated cross section for lead at 125° is $0.541\times10^{-24}~\mathrm{cm}^2/\mathrm{sr}$, with an error of about $\pm3.2\%$. If an uncertainty of ±12 eV in $(h\nu-\epsilon_K)$ due to near-edge structure is assumed for the lead foil target, the corresponding uncertainty in the calculated cross sections is about $\pm4.8\%$. Note that, without the subtraction of spurious resonances involving O and P shells, a value of $0.424\times10^{-24}~\mathrm{cm}^2/\mathrm{sr}$ was reported in Ref. [1].

The cross sections at 125° calculated according to the procedure for aluminum, gold, and bismuth are 0.001 39, 0.666, and 0.144×10^{-24} cm²/sr, respectively, instead of 1987 values of 0.001 33, 0.680, and 0.132×10^{-24} cm²/sr, respectively. The change in the value for Al is due to the current use of the DS exchange instead of the earlier KS exchange. The change in the value for gold arises from the subtraction of spurious resonances and the current choice of the DS exchange. The difference in the case of bismuth is almost entirely due to the subtraction of spurious resonances.

III. EXPERIMENTAL VALUES OF CROSS SECTIONS

As pointed out in Sec. II, the γ -ray energy was very close to the lead K-shell electron binding energy ϵ_K . So in the pulse height spectrum, elastically scattered γ rays were not resolved from lead $K\beta_2'$ x rays. Counts arising from elastic scattering were determined from the composite pulse height distribution by a least-squares fitting pro-

cedure. The fitting procedure now takes into account five $K\beta_2'$ x-ray components instead of only four employed in 1987. A reanalysis of the data obtained in the 88.03-keV experiment with lead results in nearly the same cross section, but with an error significantly larger that stated in Ref. [1]. The revised value of the lead cross section at 125° is $(0.602\pm0.091)\times10^{-24}$ cm²/sr, in excellent agreement with the new theoretical value of 0.541×10^{-24} cm²/sr.

The K-shell electron binding energy in the case of bismuth is about 90.53 keV [5,6] so 88.03-keV γ rays cannot excite K x rays in a bismuth target. However, an observation of bismuth K x rays was reported in the earlier work [1]. The production of bismuth K-shell vacancies under experimental conditions was attributed to a highenergy $\hat{\beta}$ contamination of a few percent. To our knowledge, such a contamination in a 109Cd source was not reported until then. However, recently, such a contamination was reported and traced to the presence of ¹¹³Cd with a β end-point energy of 585 keV and a half-life of 14.1 years [9,10]. Since the half-life of 109Cd is only about 463 days [7], it decays much faster than the high energy β contamination. Measurements recently made with the old source confirmed the deduced relative intensities. Additional confirmation was also obtained through measurements made with about 0.7 g/cm² aluminum absorber in front of the detector. The aluminum absorber could cut out the β rays and permit detection of a very low intensity of 264-keV γ rays from 113 Cd in addition to the 88.03-keV γ rays from ¹⁰⁹Cd.

Although we had suspected, and also reported in 1987. the high-energy β contamination, we adopted a mistakenly overcautious approach regarding some of the bismuth measurements. In particular, we only reported results of poor statistical precision obtained with a 0.139-g/cm² target, and not the more precise ones obtained with a 0.314-g/cm² target and amplifier shaping time constants varying from 1 to 3 microseconds. Since the counting rates were always less than about 125 per second, there was really no likelihood of pileup signals mimicking $K\beta'_2$ or $K\beta'_1$ x rays of bismuth. However, in the absence of any confirmation in the then-available literature of a high-energy β contamination, a suspicion of possible pileup effects unfortunately led us in 1987 to report only the thinner target results of poor precision, even though the resulting deviation from the theoretical calculation was larger than that with the three separate and more precise results obtained with the thicker target. The value of the bismuth elastic-scattering cross section at 125° turns out

to be $(0.172\pm0.017)\times10^{-24}$ cm²/sr, in reasonable agreement with the revised S-matrix value of 0.144×10^{-24} cm²/sr.

The experimental cross sections for Al and Au, unchanged since 1987, are $(0.0016\pm0.0002)\times10^{-24}$ cm²/sr and $(0.711\pm0.049)\times10^{-24}$ cm²/sr, respectively, and are in agreement with the new S-matrix calculations.

IV. CONCLUSIONS

Significant deviations previously reported between experimental and theoretical cross sections for elastic scattering of 88.03-keV γ rays through 125° have been removed (Table I). This work, and a recently reported study [3] of 81-keV γ -ray elastic scattering, show that the

S-matrix calculations in the independent-particle approximation are fairly successful in explaining γ -ray elastic-scattering cross sections even near K-shell thresholds of high-Z elements.

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- [1] P. P. Kane, G. Basavaraju, Saharsha M. Lad, K. M. Varier, L. Kissel, and R. H. Pratt, Phys. Rev. A 36, 5626 (1987).
- [2] P. P. Kane, L. Kissel, R. H. Pratt, and S. C. Roy, Phys. Rep. 140, 75 (1986).
- [3] G. Basavaraju, P. P. Kane, L. Kissel, and R. H. Pratt, Phys. Rev. A 49, 3664 (1994).
- [4] Extending the S-matrix treatment for lead by successive stages to K, K+L, K+L+M, and K+L+M+N shells, removing at each stage uncancelled spurious resonances, and adding MF contributions of remaining electrons, the cross sections for scattering of 88.03-keV γ rays through 125° by lead at the K+L and K+L+M stages were found to differ from our final value at the K+L+M+N stage by less than 2.4 and 0.6%, respectively. For the
- outermost shells with low binding energies, for which far more computer time is required, total-atom results differing by less than 0.2% are obtained when all shells are computed by S-matrix methods, since outer-shell contributions are small for this case.
- [5] Gwynn P. Williams, Electron Binding Energies for the Elements (Gordon and Breach, Switzerland, 1992).
- [6] J. A. Bearden and A. F. Burr, Rev. Mod. Phys. 39, 125 (1967).
- [7] J. Blachot, Nucl. Data Sheets 64, 913 (1991).
- [8] F. E. Bertrand, Nucl. Data Sheets B 6, 1 (1971).
- [9] H. E. Lehtihet and C. A. Quarles, Nucl. Instrum. Methods A 326, 615 (1993).
- [10] J. Liu and C. A. Quarles, Nucl. Instrum. Methods A 337, 127 (1993).