Dielectronic recombination of Pb^{79+} via high angular momenta

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We have used the AUTOSTRUCTURE code to carry out semirelativistic calculations for the dielectronic recombination of Pb^{79+} via the $2s_{1/2}-2p_{1/2}$ core excitation. We obtain excellent agreement between these semirelativistic results and measurements made at Gesellschaft für Schwerionenforschung, in particular, for the high angular momentum peak of the $2p_{1/2}20l_j$ resonances. The factor of 3 underestimate in the result for this peak that was originally obtained by Mitnik *et al.*, which has led some to conclude that only a fully relativistic approach can describe dielectronic recombination via high angular momenta in very heavy highly charged ions, are found to be in error.

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Dielectronic recombination (DR) of very heavy highly charged Li-like ions has been a testbed for experimental and theoretical studies of relativistic effects in DR [1–5]. The heavy-ion Experimental Storage Ring (ESR) at Gesellschaft für Schwerionenforschung (GSI) in Darmstadt, Germany, has been used to test quantum electrodynamics (QED) in strong fields by measuring the series of DR resonances occurring via a $2s_{1/2}-2p_{1/2}$ core excitation so as to determine the core-energy splitting to high precision [2,3]. The DR resonances themselves are particularly interesting because the relatively small $2s_{1/2}-2p_{1/2}$ energy splitting means that DR via high angular momentum states (to $l\sim 20$) makes a significant contribution to the n-resolved total.

Prior to measurements at GSI, Mitnik *et al.* [4] carried out calculations for the DR of Pb^{79+} over 0–300 eV. This covered all DR resonances that arise via the $2s_{1/2}-2p_{1/2}$ core excitation and the first ($n=6$) resonances associated with the $2s_{1/2}-2p_{3/2}$ core excitation. Multiconfiguration Dirac–Fock (MCDF) calculations were carried out for the $2p_{3/2}6l$ resonances, and for $l=0-5$ of the $2p_{1/2}nl$ resonances (for $n\geqslant 20$). The contribution from higher l for the $2p_{1/2}nl$ resonances was determined using the multiconfiguration Breit–Pauli (MCBP) semirelativistic approach incorporated within the AUTOSTRUCTURE code [6], which includes the mass–velocity and Darwin terms within the solution of the radial equations. Subsequently, measurements were made at GSI [2] for DR via the $2p_{1/2}20l$ resonances and these were found to be in good agreement with MCDF calculations [2], which were made for all l. Good agreement was found also with the MCDF results of Mitnik *et al.* [4], but the semirelativistic results reported by them were found to be a factor of 3 smaller than the measurements and MCDF results of Brandau *et al.* [2]. This led [2] to conclude that "Contributions from very high angular momenta must be included and considered in a fully relativistic framework in order to understand the dynamics involved in the DR process."

While the semirelativistic approach of AUTOSTRUCTURE cannot hope to give energy splittings to high precision in such highly relativistic systems (and so makes use of the best available N-electron energies instead [6]), its description of radiative and autoionization rates has been shown to be accurate, at least for $l=0-5$ [1]. There being no obvious reason why the semirelativistic approach should fail for high l, we have reexamined the problem. We have carried out semirelativistic calculations for all angular momenta for the DR of Pb^{79+} via the $2s_{1/2}-2p_{1/2}$ core excitation. We present our results in Fig. 1 and compare them with the measurements made at GSI [2]. We see that there is excellent agreement between the semirelativistic results from AUTOSTRUCTURE and experiment for the high angular momentum peak of the $2p_{1/2}20l_j$ resonances, at 18 eV.

The "AUTOSTRUCTURE" results shown in Fig. 1, like all such results, are actually obtained by running two codes.

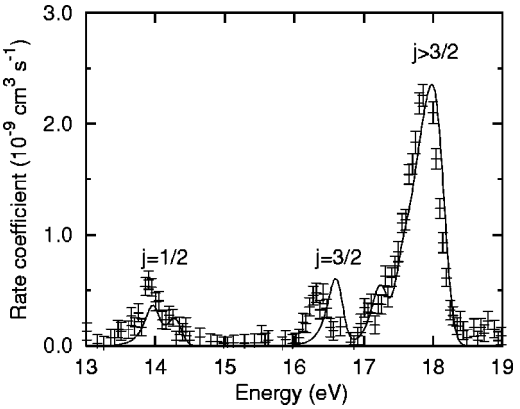

FIG. 1. DR of Pb^{79+} via $2p_{1/2}20l_j$ resonances. Solid line, semirelativistic theory (this work); experimental points, Brandau *et al.* [2]—experimental electron–ion relative velocity distribution characterized by $k_BT_{par}=0.2$ meV and $k_BT_{perp}=120$ meV.

Firstly, the main AUTOSTRUCTURE code is run to generate energy levels, autoionization rates, and radiative rates. Secondly, a postprocessor code (MDRCS12) combines this data to form DR cross sections. In addition, DR via a $2s_{1/2}-2p_{1/2}$ core excitation gives rise to a large number of outer-electron radiative stabilizing transitions of the form $n \rightarrow n'$, for $n' < 20$. The radiative rates to $n' = 2$ were determined by the main AUTOSTRUCTURE code. In the present calculation, the radiative rates to $n' > 2$ were determined hydrogenically by the postprocessor code MDRCS12. Mitnik *et al.* [4], because they were combining two sets of data from different codes, wrote a separate postprocessor code. It turns out that a factor $2J+1$, where J is the total angular momentum of the autoionizing level, was accidentally omitted when calculating the postprocessed hydrogenic radiative rates to supplement the AUTOSTRUCTURE $n \rightarrow n' = 2$ radiative data, which was used by Mitnik *et al.* [4] for $l > 5$ only. Its inclusion now gives agreement with the results, presented here, from the standard MDRCS12 postprocessor code.

Returning to Fig. 1, we see that the magnitude of the low l_j peaks (for $j = 1/2$ at 14 eV and $j = 3/2$ at 16.5 eV) is also well described by the semirelativistic approach, but the positions are not quite correct. A fully relativistic treatment of the $(N+1)$-electron energies [2,4] improves the agreement of the position of these two peaks with the observed. Finally, we note that we obtain a similar level of agreement with experiment [3] for higher members $(n > 20)$ of this series as well.

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