Erratum: State-Resolved Mutual Neutralization of Mg^+ and D^- [Phys. Rev. Lett. 128, 033401 (2022)]

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In our Letter, we reported experimental final-state distributions for Mg atoms formed in $Mg^+ + D^-$ mutual neutralization (MN) reactions at center-of-mass collision energies of 59 ± 12 meV by using the merged-beams method at the DESIREE facility at Stockholm University. In this Letter, we compared these experimental results with results from our own semiclassical calculations, based on the Landau-Zener method and a linear combination of atomic orbitals asymptotic model approach, LZ-LCAO [1], and with full-quantum (FQ) results from 2012 by Belyaev *et al.* for $Mg^+ + H^-$ MN reactions [2], $FQ_H^{(2012)}$ in the following. In this Letter, we found that the LZ-LCAO results [1] were much closer to the experimental results than $FQ_H^{(2012)}$. We used deuterium anions in the experiment, but the fact that the $FQ_H^{(2012)}$ calculations were made for Mg^+ reactions with H^- [2] cannot explain the difference. This can be seen by comparing LZ-LCAO calculations for H and D, LZ-LCAO_H and LZ-LCAO_D, as we did in Fig. 1 of our Letter and as we do in the revised Fig. 1 below.

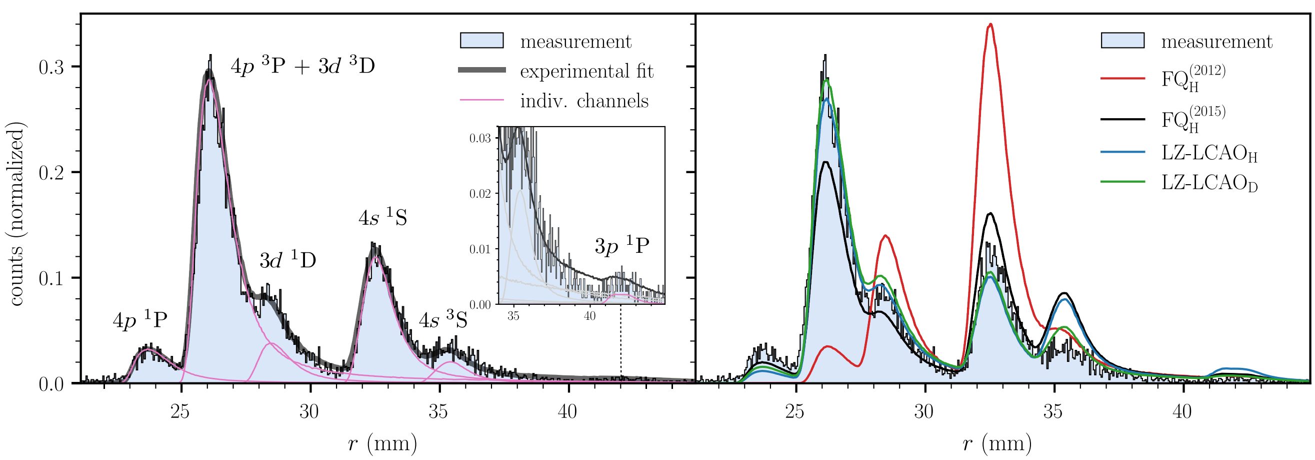

FIG. 1. Mg/D particle separation distributions, r, at $E_{CM} = 59$ meV ($E_R = 32$ meV/u) in 0.05 mm bins and normalized to unit area. Left panel: experimental data (black histogram) compared to Newtonian Monte Carlo (NMC) model data (black curve). The latter is obtained by fitting the intensities of the final $Mg(3s\,nl\ ^{2S+1}L)$ states (pink curves) to the experimental curve. The inset plot is zoomed in on the weak $3p\ ^1P^o$ channel at 42 mm. Right panel: comparison of the experimental data to synthetic NMC distributions based on the theoretical branching fractions. The red, black, and blue curves show models for neutralization of Mg^+ with H^- based on the $FQ_H^{(2012)}$, $FQ_H^{(2015)}$, and LZ-LCAO branching fractions, respectively. The green curve corresponds to neutralization with D^-, as in the present experiment, based on LZ-LCAO results. Compensation for missed MN events near the edge of the detector are included in the model results shown in the right panel (see the text for further details and definitions).

However, we were unaware of the significance of the more recent full-quantum calculation by Guitou *et al.* [3] from 2015, $FQ_H^{(2015)}$ in the following, in relation to the $FQ_H^{(2012)}$ results when our Letter was published. The $FQ_H^{(2015)}$ results are closer to the experimental results than those of $FQ_H^{(2012)}$, as can be seen in the revised Fig. 1. They are, however, still further away from the experimental data than both the $LZ\text{-}LCAO_H$ and $LZ\text{-}LCAO_D$ results.

This does not mean that LZ-LCAO gives a better or more complete description of the physics of MN reactions than full quantum mechanical treatments. Rather, it reflects how challenging FQ calculations are to carry out in practice, as exemplified by the differences between $FQ_H^{(2012)}$ and $FQ_H^{(2015)}$. Semiclassical model calculations, such as LZ-LCAO, are much easier to perform and can rather easily be extended to more complex MN reactions as, e.g., $Fe^+ + H^-$ reactions, which are important for modeling of stellar spectra [4]. We point out that the $FQ_H^{(2012)}$ results, but not the $FQ_H^{(2015)}$ results, have been extensively used as input to astrophysical modeling, even after the publication of $FQ_H^{(2015)}$. This is despite the latter predicting total MN cross sections almost twice as large as the former (and being much closer to both the $LZ\text{-}LCAO_H$ and $LZ\text{-}LCAO_D$ results). This demonstrates the crucial role that experiments like the one in this Letter have in distinguishing between different theoretical predictions.

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