

This is the accepted manuscript made available via CHORUS, the article has been published as:

## Comment II on “Topological angular momentum in electron exchange excitation of a single atom”

Klaus Bartschat and Oleg Zatsarinny

Phys. Rev. A **87**, 016702 — Published 9 January 2013

DOI: [10.1103/PhysRevA.87.016702](https://doi.org/10.1103/PhysRevA.87.016702)

# Comment on “Topological angular momentum in electron exchange excitation of a single atom”

Klaus Bartschat and Oleg Zatsarinny

Department of Physics and Astronomy, Drake University, Des Moines, Iowa 50311, USA

(Dated: May 16, 2012)

A recent article by Williams *et al.* [*Phys. Rev. A* **85** 022701 (2011)] highlights a discrepancy between experiment and theory for the linear light polarization  $P_2$  measured after impact excitation of zinc atoms by a spin-polarized electron beam. The claim is made that current collision theories must be modified by including a geometric (Berry) phase in the calculations in order to reproduce the experimental data for Zn and also similar data from the Münster group for Hg. We show that the e-Hg data can be qualitatively reproduced by our fully relativistic  $B$ -spline  $R$ -matrix approach *without* any further modification.

PACS numbers: 34.80.Dp, 34.80.Nz

A serious discrepancy between experimental data and theoretical predictions was recently reported [1] for spin-polarized electron impact excitation of the  $(4s5s)^3S_1$  state in Zn atoms. The linear light polarization  $P_2$ , measured for optical decays to the  $(4s4p)^3P_{0,1,2}$  states with a photon detector aligned along the direction of the spin polarization  $P_e$  of the incident electron beam, was found to be significantly (nearly 10% for the final state  $^3P_0$ ) different from zero while all available numerical calculations predicted an effect of less than 0.01% in the cascade-free region just above the excitation threshold. In 1982, Bartschat and Blum [2] predicted a zero result for  $P_2/P_e$  if the following assumptions are valid: i) relativistic effects, both for the projectile-target interaction and in the target structure description alone, can be neglected; ii) the orbital electronic angular momentum  $L$  and the spin  $S$  of the excited target state are well-defined, i.e., configuration interaction with terms of different  $L$  and  $S$  is negligible. The  $(4s5s)^3S_1$  state in Zn seems to be a very good candidate for such a case, and Zn is sufficiently light that spin-orbit effects during the excitation process are likely small. Hence, very small absolute values of  $P_2/P_e$  were expected, and the experimental results reported in [1] came as a major surprise.

After discussing the  $P_2/P_e$  discrepancy between theory and experiment once again for e-Zn excitation in their subsequent paper [3], to which this Comment is directed, Williams *et al.* conclude with the firm recommendation: “The task remains for theory to include a topological nondynamical phase.” No suggestion, however, is made how this might or should be done. We are not aware of any electron-atom collision theory that includes such a phase. The above statement about “theory”, however, seems to imply a view that something is missing. It is worth pointing out, therefore, that the most successful *ab initio* theories, especially those based on some variant of the close-coupling expansion for the projectile-target collision system, employ properly antisymmetrized wavefunctions for all electrons in the system, rather than the *alternative* formulation proposed by Berry and Robbins [4]. Note that Berry and Robbins themselves emphasize the *alternative* character of their

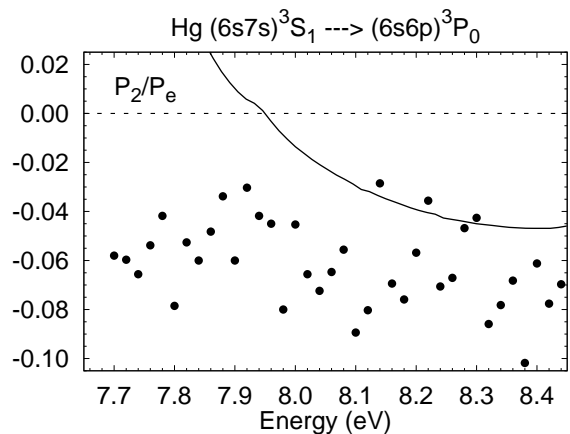


FIG. 1.  $P_2/P_e$  for spin-polarized electron impact excitation of the  $(6s7s)^3S_1$  state in Hg with subsequent optical decay to the  $(6s6p)^3P_0$  state. The experimental data of Goeke [6] are compared with the DBSR prediction based on the model described in [7].

approach. In Section 7 (page 1784) of their paper, they state that “... this [their formulation] quantum mechanics leads to the same physics (e.g. the exclusion principle) as more conventional formulations, ...”

We have no doubt that tremendous experimental effort and attention to detail was exercised in generating the experimental e-Zn results. As elaborated in [1] and [3], the data appear to be consistent against all cross checks performed to date and hence remain a mystery that we cannot explain at the present time. Figure 1, however, shows that the experimental data obtained in Münster for the e-Hg collision system nearly 30 years ago [6], which were used in [3] as further supporting evidence for the need to include a Berry-type phase, can at least be qualitatively reproduced by the DBSR model described in [7], *without* making any further changes to the method or the accompanying computer code. As seen in the figure, we obtain absolute values of up to nearly 5% for e-Hg in the cascade-free region.

We are currently investigating the dependence of these

predictions on the details of the model, in particular the description of the target structure. These calculations are extremely demanding and computationally expensive. Hence we cannot yet pinpoint to an unambiguous reason for the differences in the theoretical results for Zn and Hg. A promising candidate is a significant admixture (about 7% in the present DBSR model) of what would correspond, in a semirelativistic model, to a  $(6p^2)^3P_1$  term in the target description of the  $(6s7s)^3S_1$  state in Hg, while the respective  $(4p^2)^3P_1$  admixture to the  $(4s5s)^3S_1$  state is very small in our structure calculation for Zn. Note that such a  $^3P_1$  term would indeed violate the conditions outlined by Bartschat and Blum [2] and hence allow for a nonvanishing value of  $P_2/P_e$ .

We strongly believe that the discrepancy between theory and experiment for  $P_2/P_e$  in Zn [1] deserves further investigations on both the theoretical and experimental fronts. It seems highly advisable to independently repeat the e-Zn experiment, as unlikely as a technical problem might appear to our experimental colleagues. At the same time, we pledge to further investigate the computational model. Furthermore, while performed with a state-of-the-art apparatus nearly thirty years ago, the

Münster group never published their  $P_2/P_e$  data for this particular process in Hg. Hence, we recommend checking those data as well using the best available experimental methods today. In particular, the finite energy resolution might partly explain the major discrepancies in Fig. 1 between the experimental data and the DBSR predictions in the near-threshold region where the cross section, and hence the signal, is very small. Other targets such as Cd (poisonous and hence experimentally challenging but certainly not impossible) or other quasi-two-electron systems (Yb or alkaline-earth metals) come to mind. While we remain open to the possibility of something being still missing in our, and presumably other current theoretical models for e-Zn collisions, we are convinced that the resolution of the discrepancy does not, and should not, involve modifying our approach by introducing the Berry phase in an *ab initio* formulation that already accounts for the Pauli Principle to full extent.

This work was supported by the United States National Science Foundation under grants PHY-0903818 and PHY-1068140. One of us (KB) would like to sincerely thank Jim Williams and his group for many stimulating discussions on this problem during the past nearly 10 years.

- 
- [1] L. Pravica, J. F. Williams, D. Cvejanović, S. Samarin, K. Bartschat, O. Zatsarinny, A. D. Stauffer, and R. Srivastava, *Phys. Rev. A* **83** (2011) 040701
  - [2] K. Bartschat and K. Blum, *Z. Phys. A* **304** (1982) 85.
  - [3] J. F. Williams, L. Pravica, and S. Samarin, *Phys. Rev. A* **85** (2012) 022701
  - [4] M. V. Berry and J. M. Robbins, *Proceedings of the Royal Society of London A* **453** (1997) 1771.
  - [5] O. Zatsarinny and K. Bartschat, *Phys. Rev. A* **77** (2008) 062701.
  - [6] J. Goeke, PhD Thesis, University of Münster (Germany), unpublished (1983).
  - [7] O. Zatsarinny, and K. Bartschat, *Phys. Rev. A* **79** (2009) 042713.