

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

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In their recent paper, Williams *et al.* [*Phys. Rev. A* **85**, 022701 (2012)] report on the apparatus and experimental method for the measurement of the Stokes parameter  $P_2$  associated with spin-polarized electron impact ( $3d^{10}s^2$ )  $^1S_0 \rightarrow (3d^{10}4s5s)$   $^3S_1$  excitation of zinc. On the basis of a qualitative semiclassical argument, they make the following claim regarding the discrepancy between theory and experiment for  $P_2$ : “The task remains for theory to include a topological nondynamical phase.” We analyze the validity of this assertion.

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Discrepancies between theories and experiment are the hallmark of progress in physics. The past two decades have seen immense progress in the theoretical understanding of electron-atom collisions. Excitation and ionization processes are now able to be routinely calculated utilizing recently developed advanced theoretical methods [1–5]. Some of these techniques have also been shown to work very well in the fully relativistic domain [6,7]. Together, these methods have resolved many long-standing discrepancies between theory and experiment.

Recently, Pravica *et al.* [8] have outlined the experimental method for the measurement of the  $P_2$  Stokes parameter associated with spin-polarized electron-impact ( $3d^{10}s^2$ )  $^1S_0 \rightarrow (3d^{10}4s5s)$   $^3S_1$  excitation of zinc. The light polarization, measured for the optical decay to the  $(4s4p)$   $^3P_{0,1,2}$  states, was found to be significantly different from zero (nearly 10% for the final  $^3P_0$  state) in the cascade-free region just above the excitation threshold, whereas, all presented calculations predicted less than 0.01%. Using the relativistic convergent close-coupling (RCCC) method [9] with the state multipole theory of Bartschat *et al.* [10], we also obtain near 0% for  $P_2$  in consistent agreement with  $R$ -matrix and relativistic distorted-wave theories [8].

Williams *et al.* [11] suggest that the electron-atom collision theories neglect the “geometric exchange angular momentum” that is utilized in the paper of Berry and Robbins [12] by stating “Electron quantum scattering theories use antisymmetrized wave functions, but none include this geometrical exchange angular momentum.” Furthermore, they suggest “the nonzero  $P_2$  values are interpreted as consequences of the rotational motion of the exchanged electron spin causing an effective angular momentum associated with the spin-orbit interaction.” We address these two statements below.

Berry and Robbins [12] explicitly state that their method of employing a transported spin basis that exchanges the spins along with the positions, rather than a fixed spin basis, produces exactly the same results as conventional quantum mechanics. A verbatim quote from their conclusion reads:

“... this quantum mechanics leads to the same physics (e.g., the exclusion principle) as more conventional quantum mechanics.”

Therefore, it would be inconsistent for any scattering theory to employ both antisymmetric wave functions *and* a transported spin basis because they are two separate and distinct means to achieve a phase change of  $(-1)$  in the exchange of two spin-1/2 particles. To employ both methods would lead to a destruction of the wave function’s symmetry properties, which enforce the Pauli exclusion principle.

The spin-orbit interaction, Darwin term, and relativistic mass corrections all follow from the nonrelativistic limit of the Dirac equation. In the RCCC method, which is entirely based on the Dirac equation, we are not free to insert extra *ad hoc* spin-orbit interaction terms. Furthermore, applications of the Dirac equation to semiclassical [13,14] and nonrelativistic limits [15,16] of electron dynamics have indicated the *emergence* of geometric phases in the dynamics. For example, Mathur [15] highlights that: “The spin-orbit interaction is shown to arise as a Berry phase term in the adiabatic effective Hamiltonian for the orbital motion of the Dirac electron.” In a similar vein, Shankar and Mathur [16] report that: “The Thomas precession in the nonrelativistic limit of the Dirac equation may be attributed to a non-Abelian Berry vector potential.” The important point to draw from these papers is that the geometric phase dynamics *emerge* from the Dirac equation in various nonrelativistic and semiclassical approximations. It would be erroneous to insert extra geometric phase terms into *ab initio* scattering theories based on the Dirac equation.

Berry’s review articles [17,18] clearly demonstrate the importance of accounting for phases when the parameters of a quantum-mechanical wave function are slowly cycled around a circuit. However, the essential theme across many areas of physics is that geometric phases arise naturally from the underlying equations describing the phenomena. For example: (i) Berry [19] highlights that his geometric phase approach for the well-known Aharonov-Bohm effect [20] can be shown to be equivalent to that obtained by properly incorporating the vector potential  $\mathbf{A}$  into the Schrödinger equation. (ii) In analyzing the cyclic changes in the polarization of light traversing twisted dielectrics, Berry [21] shows that the geometric phase manifesting itself can be derived from Maxwell’s equations. Likewise, the geometric phases that manifest in light propagating through twisted optical fibers [22,23] can be explained using classical electrodynamics (Maxwell’s equations) by integrating the parallel transformation of the electric-field vector inside the optical fiber [24].

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Geometric phases play an important role across many areas of physics, however, they emerge naturally from *ab initio* methods based on the appropriate equations, such as the Dirac equation, Maxwell's equations, or the Schrödinger equation. The discrepancy between theory and experiment for the zinc  $P_2$  Stokes parameter measurement [8] will require further investigations on both the theoretical and the experimental fronts, but the resolution to the discrepancy does not involve

modifying the fundamental equations of quantum electrodynamics with geometric phases. The latter emerge from the former.

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