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High-precision atomic calculations using the relativistic all-order method: including triple excitations EUGENIYA ISKRENOVA-TCHOUKOVA, MARIANNA S. SAFRONOVA, Department of Physics and Astronomy, University of Delaware — High-precision atomic calculations combined with experiments of matching accuracy provide an excellent opportunity to improve our understanding of atomic structure as well as to test atomic theory. One very appealing and challenging application of such calculations is the study of parity nonconservation (PNC) in atoms and ions. It requires a systematic study and accuracy estimates of the PNC amplitude and other atomic parity conserving quantities. While the implementation of the relativistic all-order method that completely includes single and double excitations yielded very accurate data for some atomic properties, the results for a number of atomic properties where the correlation was very large were much less accurate. The partial inclusion of the triple excitations, where only energy and single excitation coefficient equations were modified, provided improved accuracy for certain cases where specific contributions were dominant but produced inconsistent results in other cases. This work is aimed at the consistent inclusion of the triple excitations. We evaluate computational challenges involved in the efficient implementation of the all-order method with triple excitations balancing the need for accurate calculation and computational difficulties associated with an extremely large number of the corresponding triple excitation coefficients.

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