Implementations of the Levin-Weniger convergence accelerator and applications to problems in physics

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Abstract

Levin sequence transformations [1] as generalized in [2], are useful tools for the summation of slowly convergent series appearing in atomic variational calulations (as an example, see [3]). The necessity of high precision results for the upper bound estimates has the consequence of dealing with a high number of summations that have to be done accurately. Therefore, special care must be paid in the balance between precision and computational time.

For the numerical series that appear in the evaluation of the multi-electron integrals required, it is not known a general expansion for large n of the difference between the infinite and the partial sum up to n. The generalized Levin formula for the convergence acceleration requires a choice for the remainder estimates ω_n. In this work we will propose and additional choice of ω_n which comes from the use of the Euler-McLaurin formula for series for which the general term behaves asymptotically as $n^{-\alpha}$ and compare to the Levin *u*-transform for different types of series of physical interest. In particular, we will find some examples where the present choice is exact.

In addition to this, two strategies will also be presented in this work for reducing the welll known unstabilities of the convergence accelerators due to precision losses: (i) using a rearrangement of terms for the numerical evaluation and (ii) by means of an arbitrary precision implementation of the Levin sequence transformation in C++ using a free multiprecision library (MPFR). Some numerical tests will be shown.

References

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[3] I. Porras and F.W. King, *Evaluation of some integrals for the atomic three-electron problem using convergence accelerators*, Phys. Rev. A **49**, 1637 (1994).