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## Very Precise Atomic Structure Calculations for the Determination of Atomic Parity Non-Conservation

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### Abstract

Atomic physics is still at the frontier of our exploration of fundamental physical laws. For example, the comparison of the theoretical and experimental values of the atomic parity non-conservation (PNC) amplitude, which, as we will show, arises from Glashow-Weinberg theory of electroweak interactions, constitutes one of the most stringent tests of the Standard Model. By reviewing current theoretical and experimental data, we will see, however, that the theoretical results lag behind the latter. Moreover, there are several calculations on the cesium atom, for example, that differ at a sub-percentage level.

There are two main obstacles inherent in any precise atomic structure calculation: first, the determination of an optimal radial basis and a numerically stable evaluation of atomic integrals, and second, the question of how to take into account electron correlation. We describe our solution of the former [1] and our current efforts for solving the latter [2].

The optimal radial basis are the Sturmian functions. They are orthonormal, discrete and complete on infinite interval. The problem of the numerical stability is solved by considering Sturmian functions not “analytically”, i.e. through their explicit functional form, but “algebraically”, i.e. as functions satisfying certain recursion relations. These recursion relations then imply recursion relations for the integrals of these functions.

The electron correlation in closed-shell atoms can be accurately accounted for by the coupled-cluster method. In the case of open-shell atoms, one can use a combination of coupled-cluster and configuration interaction methods. We describe the adaptation of these methods to the spherical symmetry of the atoms.

[1] T. Uhlířová, J. Zamastil, and J. Benda, *Comput. Phys. Commun.* **280**, 108490 (2022).

[2] T. Uhlířová and J. Zamastil, in progress.

ההרצאה תתקיים ביום רביעי, ה-22.9.21 בשעה 12:30

באודיטוריום המכון למצב מוצק, קומת כניסה

The lecture will take place on Wednesday, 21.9.22 at 12:30  
at the Solid State Institute Auditorium, entrance floor

Host: Assistant Professor Yuval Shagam