La boite à outils de l'algèbre extérieure pour le problème à N-corps fermionique

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Résumé

It has been argued by Valatin in 1951 that the exterior algebra is the natural mathematical framework for the N-body problem of identical Fermionic particles [1]. However, the tools developed in this mathematical field [2] have remained little exploited up to now in quantum physics. It is the purpose of this talk to review some of the key exterior algebra concepts and techniques that we find particularly relevant for physicists and chemists.

We will focus on the concept of p-internal space and the derived one of porthogonality [3], which generalizes that of strong-orthogonality and can be viewed as a graded indistinguishability measure for electronic states. p-orthogonality has been applied in the past to constrain geminal models [4], and work in progress shows that computational cost can be drastically reduced by using new geminal ansätze based on such algebraic constraints.

Time permitting, we will show the connection between the concept of "cancelator space" and Configuration Interactions with arbitrary reference wave functions.

References

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Mots-Clés: algèbre extérieure

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