Many-body perturbation theories in modern quantum chemistry and nuclear physics

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I. SCOPE

The scope of the proposed interdisciplinary workshop is to bring together researchers from quantum chemistry and nuclear physics to elaborate on the use of many-body perturbation theories (MBPT) for the description of fermionic many-body quantum systems.

A. Perspective on single-reference MBPT in quantum chemistry and nuclear physics

Even though pioneering formal development was performed in nuclear physics [1–5], MBPT was truly developed in quantum chemistry. First applications of single-reference (SR) MBPT were performed for the description of *weak correlation* effects in closed-shell systems. These weakly correlated systems have the particularity of being qualitatively well represented by an uncorrelated Hartree-Fock (HF) Slater determinant, which is then used as a starting point for the perturbative expansion of the wave function. Even if its application is restricted to closed-shell non-degenerate ground states, the SR-MBPT can be considered as one of the most important contributions to the quantum many-body problem, as it has led to very important progresses in both fundamental and applied branches of this broad field of research. Regarding its fundamental aspects, SR-MBPT can be thought as a very powerful guide for the development of many-body methods, as it consists in a set of *constructive* equations allowing to *systematically* improve the description of the many-body wave function. One of the most important results of the SR-MBPT is the so-called linked-cluster theorem [1, 2] which established the conditions guaranteeing the extensive character of the approximate energy, which is a fundamental property of many-body systems. An important consequence of this theorem is the *product-structure* of the many-body wave function, which has lead to the development of one of the most accurate and efficient methods in quantum chemistry, the so-called Coupled-Cluster (CC) theory [6]. In addition

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to these great successes in the fundamental understanding of the many-body problem, SR-MBPT is also a powerful tool to obtain a good compromise between accuracy and computational cost. The most popular version of SR-MBPT is certainly the so-called Møller-Plesset at second order (MP2) [7] that combines moderate computational scaling, the fundamental property of extensivity of the energy together with a reasonable accuracy (better than some CC expansions in many cases). The generalization of these ideas to high-spin non-degenerate open-shell ground states has been introduced in several forms, the most popular being certainly the use of symmetry-broken wave functions (unrestricted HF). Furhermore, SR-MBPT has been used to correct non-perturbative methods in an optimal way, i.e., perturbative corrections to CC theory have produced the "gold standard" of quantum chemistry for SR-type problems under the form the so-called CCSD(T) method [8] and have led to even more advanced approximations [9].

As the equations associated with SR-MBPT (and SR methods in general) are well established, current developments involving SR-MBPT in quantum chemistry go in two main directions

- treating larger systems [10–15] thanks to the local character of electronic correlations [16],
- reducing the error due to the use of finite basis sets via the use of geminal functions [17–20] (F12-MP2).

Thanks to these developments, the MP2 method is nowadays applicable to systems made out of several thousands of atoms [21], and the rapid development of F12-MP2 allows one to push the boundaries of the applicability domain of such a method.

Despite its great success in quantum chemistry, MBPT has only been rarely applied as a standalone approach to the nuclear many-body problem. Initially, the hard-core nature of the nuclear Hamiltonian led to singularities in the perturbative expansion that needed to be dealt with from the outset, e.g. via the non-perturbative Brueckner theory essentially based on the resummatrion of particle-particle ladders to all orders [5]. In recent years, a more convincing, systematic and practical approach has consisted in taming down the strong short-range repulsion of inter-nucleon interactions via, e.g., unitary free-space Similarity Renormalization Group (SRG) transformations of the Hamiltonian [22]. Even though the advent of renormalized nuclear interactions authorizes SR-MBPT to compete in closed-shell nuclei with state-of-the-art non-perturbative methods, i.e., CC [23], self-consistent Green's functions (SCGF) [24, 25] or in-medium similarity renormalization group (IM-SRG) [26] techniques, at only a fraction of the computational costs [27], SR-MBPT has only been seldom used in the nuclear context so far [27–29].

B. Strongly correlated systems

Beside the success of SR methods for non-degenerate electronic systems (mainly organic chemistry), it was recognized quite early that in many important chemical situations (bond-stretching, excited-states, transition metal complexes, low-spin open-shell systems) such a treatment was inadequate and the correlation problem requires a more general ansatz for the wave function. Since the 1980s, a large activity has been then devoted to the development of multi-reference (MR) theories with the aim of describing systems that cannot be qualitatively represented by a unique Slater determinant, i.e., so-called *strongly correlated systems*. The intrinsic MR character of certain quantum systems is not restricted to the field of atomic or molecular physics but is also found for singly- and doubly-open shell systems far away from magic shell closures [30].

It could be thought that the core ideas underlying SR-MBPT would be easily generalized to the MR problem, but the number of different MR methods (and acronyms) along with their varying quality from one system to another demonstrate the contrary. At the heart of the difficulties encountered for MR systems lies a complex zeroth-order wave function that is composed of several *reference determinants*. Most exotic physical properties of strongly correlated systems mainly depend on the ratio of the coefficients of these reference determinants. The specificities of strongly correlated systems translates into the complexity of the Hamiltonian matrix expressed within the set of these reference determinants, exhibiting near energetic degeneracies and/or large interactions. In most cases, this complexity arises from a relatively small number of *strongly correlated* particles, meaning that the number of reference determinants is small enough to allow for a non-perturbative treatment, thus avoiding divergence problems. Nevertheless, to achieve a quantitative description of the system, weak correlation effects involving all other particles must be treated, as in the SR case. These effects require the inclusion of other Slater determinants, the so-called *external determinants*, which are in general much higher in energy than the reference ones. Consequently, MR problems involve physical effects from different energy scales.

C. Cross-disciplinary perspectives of state-of-the-art developments

Unlike in the SR case, there are no well established MR-MBPT or MR-CC equations. Nevertheless, powerful theories have emerged in quantum chemistry to deal with situations where the coupling between reference and external Slater

determinants is relatively weak. The most popular methods are the complete active space PT2 (CASPT2) [31] and the N-electron valence PT2 (NEVPT2) [32, 33]. They are known to be rather robust and are nowadays used routinely for systems involving several hundreds of electrons. Current developments in these directions also consist in treating larger systems and reducing the basis set error. It is one of the main aims of the present workshop to expose the nuclear physics community to these well-established quantum chemistry methods in order to see whether the description of atomic nuclei could benefit from them.

There are, nonetheless, many cases in chemistry where the coupling between reference and external determinants is so large that there is a qualitative change in the composition of the zeroth-order wave function, and, consequently, of the physical properties of the system. This can be understood as a drastic change of the interaction within the reference space under the effect of the external one. Taking this effect into account at the perturbative level is not straightforward, unless one uses the framework of the so-called dressed or effective Hamiltonian that has been initially developed in nuclear physics [34, 35]. Different formalisms have emerged in quantum chemistry [36–44], but most of them face two problems: divergences caused by low-lying excited states and/or the loss of the extensivity property of the energy. Very recently an alternative method has been proposed [45] to bypass these two problems that shows encouraging results.

In recent years the use of symmetry-broken reference states has added a new flavour to the treatment of near-degenerate quantum systems. The most important examples relate to the breaking of global gauge (U(1) group) and/or rotational (SU(2) group) symmetries associated with the conservation of particle-number and total angular-momentum. While initially developed in connection with SCGF [25, 46] and CC [47] theories, the transfer to MBPT is under current investigation [48]. Still, the spontaneous breaking of the symmetry is only an intermediate artefact in finite quantum systems used to commute the degeneracy with respect to particle-hole excitations into a degeneracy with respect to symmetry transformations. Eventually, symmetries must be restored in order for the targeted eigenstates to carry good quantum numbers. While the restoration of symmetries based on projection techniques has a long history when performed on top of a mean-field wave-function, it is only recently that it has been consistently formulated in connection with symmetry-unrestricted CC [49–51] and MBPT [49, 50] theories. *Ab initio* applications based on realistic nuclear Hamiltonians remain to be performed in order to judge the merit of these novel many-body approaches to consistently handle strong and weak correlations in (near) degenerate systems. The experience of quantum chemists with the potential benefit of breaking and restoring symmetries being quite moderate[51], it is one of the main objectives of the present workshop to bring these ideas and methods to their full attention.

Beyond the extension of innovative MR-MBPT flavours with genuine open-shell capabilities, the efficient implementation is key for further advancing an ab initio treatment to larger systems and basis sets. With the aid of novel data-compression techniques and efficient tensor-factorization algorithms the computational cost can be reduced to a minimum [52]. While these have become standard tools in quantum chemistry and solid state physics the transfer to the realm of nuclear structure remains yet to be performed. In particular the multi-body nature of the strong interaction motivates the adaption of similar techniques to operators of higher particle rank, e.g., in the context of high-order singular-value decompositions.

II. GOALS OF THE WORKSHOP

In summary, the goals of the workshop are to

1. educate nuclear physicists about the relevance of MBPT methods in modern quantum many-body calculations.
2. exchange ideas regarding state-of-the-art MBPT methods between quantum chemists and nuclear physicists.
3. identify the systems, observables and situations for which perturbative methods are appropriate.
4. discuss the merits and the efficiency of the various strategies to treat near-degenerate and degenerate systems via perturbative methods.

In order to facilitate the understanding and involvement of young theorists and experimentalists as well as to lay a common ground for quantum chemists and nuclear theorists, five 1h15mns lectures on (i) the fundamentals of many-body perturbation theory, (ii) the historical trends and future directions of MBPT, (iii) the introduction to multi-reference approaches, (iv) the concept of symmetry breaking and restoration in the context of MBPT and (v) basic properties of nuclear interactions in connection to MBPT calculations, will be given at the beginning of the workshop.

A. Introductory lectures

1. P. Piecuch *Introduction to single-reference many-body perturbation theory and its diagrammatic representation*
2. R. Roth *Nuclear interactions and many-body perturbation theory: convergence, accuracy and sensitivity*
3. C. Angeli *Basics of multi-reference many-body perturbation theories*
4. T. Duguet *Basics of symmetry broken and restored many-body perturbation theory*

B. List of presentations

1. Application of MBPT to closed-shell systems
   - C. Drischler *Many-body perturbation theory calculation of infinite nuclear matter at zero temperature*
   - F. R. Xu *Many-body perturbation theory calculations of closed-shell nuclei*
   - D. Tew *Explicitly correlated Møller-Plesset perturbation theory*
   - P. Piecuch *Perturbative corrections to non-perturbative methods*
   - C. Wellenhofer *Many-body perturbation theory calculation of infinite nuclear matter at finite temperature*
   - F. Hummel *Observable calculation in zero and finite-temperature many-body perturbation theory*
2. MBPT methods for (near-)degenerate systems
   - A. Tichai *Multi-configuration perturbation theory for open-shell nuclei*
   - E. Giner *A Jeziorski-Monkhorst fully uncontracted multi-Reference perturbative treatment*
   - P. Arthuis *Bogoliubov many-body perturbation theory for open-shell nuclei*
   - Y. Guo *Explicitly correlated NEVPT2*
3. Resummation of perturbation series
   - O. Costin *Different methods to turn a divergent series into a convergent one*
   - J. Toulouse *Review of several formulations and variants of the random-phase approximation*
4. Computational advances in MBPT
   - Q. Ma *Exploiting pair natural orbitals for linear scaling MP2*
5. Some new non-perturbative flavor(s)
   - G. Scuseria *Symmetry, degeneracy, and strong correlation*

C. Schedule

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	Monday		Tuesday	Wednesday	Thursday	Friday
09h45	Welcome					
10h00	**Piecuch**	9h30	**Xu**	**Wellenhofer**	**Costin**	**Guo**
11h00	Break	10h30	Break	Break	Break	Break
11h30	**Piecuch**	11h00	**Tew**	**Piecuch**	**Arthuis**	**Ma**
12h30	Lunch	12h00	Lunch	Lunch	Lunch	Lunch
14h00	**Roth**	14h00	**Drischler**	**Toulouse**	**Giner**	
15h15	Break	15h00	Break	Break	Break	
15h30	**Angeli**	15h30	**Hummel**	**Scuseria**	**Tichai**	
16h45	**Duguet**	16h30	Discussions	Discussions	Discussions	
18h00	End	18h00	End	End	End	
		20h00		Social dinner		

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