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Advances in Many-Body Perturbation Theory for Closed- and Open-Shell Nuclei

It is one of the ultimate goals of theoretical nuclear physicist to calculate properties of atomic nuclei starting from realistic internucleon interactions. For light nuclei, the exact diagonalization of the Hamiltonian matrix in a sufficiently large Hilbert space, namely the no-core shell model [1], is able to provide very accurate calculations. However, when dealing with not very light nuclei, the size of the Hilbert space quickly becomes intractable. Therefore, specific many-body methods should be developed to surmount this problem. One strategy is to project the Schrödinger equation into a small model space, called P-space, by constructing an effective Hamiltonian, and then to solve the Schrödinger equation in the P-space.

In this talk we describe many-body perturbation theory (MBPT) as an approach to compute such effective Hamiltonians [2, 3], applicable for both closed-shell nuclei and open-shell nuclei (i.e., the valence-space effective Hamiltonian for the nuclear shell model calculation). The main goal is to incorporate effectively the information on nucleonic excitations from the excluded part of the Hilbert space (the complement of the P-space) into the P-space. I will present new developments of MBPT performed within both Brillouin-Wigner (BW) and Rayleigh-Schrödinger (RS) formalisms.

Although the BW perturbation series contains the undesired energy dependence, it has a simple algebraic structure. A novel approach is proposed [2] to efficiently perform iterative calculations and study the order-by-order convergence of MBPT in powers of the nucleon-nucleon interaction. Analytic calculations show that we can always make the BW perturbation series for the nuclear ground state converging (independently of the choice of the nucleon-nucleon interaction or the choice of the nucleon-site calculations) due to the variational principle. Numerical calculations for 4He, 16O and some selected p-shell nuclei with a new K-box iterative method confirm this finding.

RS MBPT in the diagrammatic representation is widely applied to nuclear ground-state calculations [4] and effective-Hamiltonian constructions for the nuclear shell model [5]. However, existing applications of this diagrammatic method usually stop at 3rd order, because of the prohibitive number of diagrams involved at higher orders. We advance this diagrammatic formulation of RS MBPT beyond the conventional 3rd order, by implementing automatic generation and evaluation of Feynman-Goldstone diagrams. This allows us to compute nuclear ground states up to 6th order and derive valence-space effective Hamiltonians up to 5th order. We believe that these developments build further the path to ab-initio description of atomic nuclei.

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Zhen Li and Nadezda A. Smirnova. Converging Many-Body Perturbation Theory for Ab Initio Nuclear-Structure: I. Brillouin-Wigner Perturbation Series for Closed-Shell Nuclei. arXiv:2306.13629 (2023).
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[4] Alexander Tichai, Robert Roth, and Thomas Duguet. Many-body perturbation theories for finite nuclei. Front. Phys. 8, 164 (2020).

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