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Padé-resummed high-order perturbation theory for nuclear structure calculations

Robert Roth *, Joachim Langhammer

Institut für Kernphysik, Technische Universität Darmstadt, Schlossgartenstr. 9, 64289 Darmstadt, Germany

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ABSTRACT

We apply high-order many-body perturbation theory for the calculation of ground-state energies of closed-shell nuclei using realistic nuclear interactions. Using a simple recursive formulation, we compute the perturbative energy contributions up to 30th order and compare to exact no-core shell model calculations for the same model space and Hamiltonian. Generally, finite partial sums of this perturbation series do not show convergence with increasing order, but tend to diverge exponentially. Nevertheless, through a simple resummation via Padé approximants it is possible to extract rapidly converging and highly accurate results for the ground-state energy once perturbative contributions beyond 5th order are included.

1. Introduction

The treatment of the nuclear many-body problem is a central and long-standing issue in nuclear structure theory. Ideally, we would like to solve the many-body problem *ab initio*, i.e., starting from a given nuclear Hamiltonian without any conceptual approximations. With the advent of high-precision nuclear potentials that are based systematically on Quantum Chromodynamics (QCD) through chiral effective field theory [1,2], the demand for exact *ab initio* solutions of the nuclear many-body problem has grown. Only these schemes establish a rigorous and quantitative connection between nuclear structure observables and the underlying QCD input.

The no-core shell model (NCSM) is one of the most universal exact *ab initio* methods, which gives access to all aspects of nuclear structure [3–5]. Other methods, are either restricted to certain classes of Hamiltonians, like the Green's Function Monte Carlo approach [6], or they are limited to certain nuclei and observables, like the coupled-cluster approach [7]. All of them are computationally demanding, which leads to a severe limitation regarding the number of nucleons that can be handled.

Therefore, approximate many-body schemes using the same Hamiltonians, i.e. approximate *ab initio* methods, also provide indispensable information. In particular approaches that use controlled and systematically improvable approximations are of great practical importance. In this category, many-body perturbation theory (MBPT) is one of the most powerful and widely used methods. On the one hand, the evaluation of low orders of perturbation theory is computationally simple and can be done for the whole nuclear mass range [8–11] as well as for infinite nuclear matter [12]. On the other hand, it is deemed systematically improvable, either by extending the MBPT calculations order-by-order or by using infinite partial summations, like ladder- or ring-type summations [13–15]. However, the accuracy of low-order perturbative estimates, e.g. for ground-state energies, or possible extensions of the MBPT series to higher orders and the resulting convergence pattern are rarely, if ever, addressed in the nuclear structure context.

In this Letter, we apply MBPT for the calculation of the ground state energy of several closed-shell nuclei. We extend the order-by-order calculation of the perturbative energy contributions up to 30th order, study the convergence behavior, and compare to exact NCSM calculations for the same Hamiltonian and model space. We introduce Padé approximants as a highly efficient tool for the resummation of the divergent power-series of MBPT into a rapidly converging series and demonstrate their accuracy for the description of ground-state energies at sufficiently high orders.

2. Many-body perturbation theory

2.1. Formalism

We aim at a perturbative expansion of the many-nucleon Schrödinger equation

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle \tag{1}$$

for the translational invariant nuclear Hamiltonian $H = T - T_{\rm cm} + V$, where we assume V to be a two-body interaction for

* Corresponding author.
E-mail address: robert.roth@physik.tu-darmstadt.de (R. Roth).

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simplicity. In a first step we have to chose the unperturbed basis, which in turn defines the unperturbed Hamiltonian. From the practical point of view, a basis of Slater-determinants constructed from a set of single-particle states is most convenient. The underlying single-particle basis will typically be a Hartree–Fock or a harmonic oscillator basis—for simplicity we assume the latter. The unperturbed Hamiltonian H_0 is a one-body operator containing the kinetic energy T and a harmonic oscillator potential. The unperturbed Slater determinants $|\Phi_n\rangle$ fulfill the eigenvalue relation

$$H_0|\Phi_n\rangle = \epsilon_n|\Phi_n\rangle \tag{2}$$

with eigenvalues ϵ_n being the sum of the single-particle energies of the occupied states. After the unperturbed Hamiltonian is fixed, the perturbation is defined through $W = H - H_0$. This partitioning leads to the Møller–Plesset formulation of MBPT and obviously other partitionings of the Hamiltonian are possible [16,17]. For ease of presentation, we assume that the unperturbed state corresponding to the eigenstate we are interested in is non-degenerate, as it is the case for the ground state of closed shell nuclei. In the case of degeneracy, as e.g. for the excited states of closed shell nuclei, one would have to diagonalize the full Hamiltonian in the degenerate subspace and pick the eigenstates with the desired quantum numbers as unperturbed states.

The standard Rayleigh–Schrödinger perturbation series can now be constructed based on a Hamiltonian (using the notation from Ref. [17])

$$H(\lambda) = H_0 + \lambda W \tag{3}$$

containing an auxiliary expansion parameter λ that continuously connects the unperturbed Hamiltonian $H_0 = H(\lambda = 0)$ with the full Hamiltonian $H = H(\lambda = 1)$. The energy eigenvalues $E_n(\lambda)$ and the corresponding eigenvectors $|\Psi_n(\lambda)\rangle$ of $H(\lambda)$ are formulated as a power series in λ

$$\begin{aligned} E_n(\lambda) &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots, \\ \big|\Psi_n(\lambda)\big\rangle &= \big|\Psi_n^{(0)}\big\rangle + \lambda\big|\Psi_n^{(1)}\big\rangle + \lambda^2\big|\Psi_n^{(2)}\big\rangle + \cdots. \end{aligned} \tag{4}$$

In the absence of degeneracy the lowest-order contributions are simply given by the unperturbed quantities, i.e.,

$$E_n^{(0)} = \epsilon_n, \qquad \big|\Psi_n^{(0)}\big\rangle = |\Phi_n\rangle. \tag{5}$$

Inserting the Hamiltonian (3) and the power series (4) into the Schrödinger equation (1) leads to the fundamental equation

$$\begin{aligned} &H_0\big|\Psi_n^{(0)}\big\rangle + \sum_{p=1}^{\infty}\lambda^p\big(W\big|\Psi_n^{(p-1)}\big\rangle + H_0\big|\Psi_n^{(p)}\big\rangle\big) \\ &\quad = E_n^{(0)}\big|\Psi_n^{(0)}\big\rangle + \sum_{p=1}^{\infty}\lambda^p\left(\sum_{j=0}^{p} E_n^{(j)}\big|\Psi_n^{(p-j)}\big\rangle\right). \end{aligned} \tag{6}$$

Assuming that the unperturbed states form an orthonormal basis and using the intermediate normalization $\langle\Psi_n^{(0)}|\Psi_n(\lambda)\rangle = 1$ we obtain $\langle\Psi_n^{(0)}|\Psi_n^{(p)}\rangle = 0$ for $p > 0$, which allows us to project-out all required information on the individual contributions in the power series. By multiplying Eq. (6) with $\langle\Psi_n^{(0)}|$ and matching same orders of λ on both sides, we immediately obtain a simple expression for the pth-order energy contribution

$$E_n^{(p)} = \big\langle\Psi_n^{(0)}\big|W\big|\Psi_n^{(p-1)}\big\rangle. \tag{7}$$

By multiplying Eq. (6) with $\langle\Psi_m^{(0)}|$ with $m \neq n$ and matching λ-orders, we obtain an expression for the amplitudes

$$\begin{aligned} C_{n,m}^{(p)} &= \big\langle\Psi_m^{(0)}\big|\Psi_n^{(p)}\big\rangle \\ &= \frac{1}{E_n^{(0)} - E_m^{(0)}}\left(\big\langle\Psi_m^{(0)}\big|W\big|\Psi_n^{(p-1)}\big\rangle - \sum_{j=1}^{p} E_n^{(j)}\big\langle\Psi_m^{(0)}\big|\Psi_n^{(p-j)}\big\rangle\right) \end{aligned} \tag{8}$$

which characterize the perturbative corrections to the eigenstates $|\Psi_n^{(p)}\rangle$ expanded in the unperturbed basis

$$\big|\Psi_n^{(p)}\big\rangle = \sum_m C_{n,m}^{(p)}\big|\Psi_m^{(0)}\big\rangle \tag{9}$$

with $C_{n,n}^{(p)} = 0$ for $p > 0$ and $C_{n,m}^{(0)} = \delta_{n,m}$.

We can cast Eqs. (7) and (8) into a more transparent form by systematically introducing the amplitudes $C_{n,m}^{(p)}$ and formulating all matrix elements in terms of the unperturbed states. For the pth-order energy contribution we obtain

$$E_n^{(p)} = \sum_m \langle\Phi_n|W|\Phi_m\rangle C_{n,m}^{(p-1)}. \tag{10}$$

Similarly we obtain for the pth-order amplitudes

$$C_{n,m}^{(p)} = \frac{1}{\epsilon_n - \epsilon_m}\left(\sum_{m'}\langle\Phi_m|W|\Phi_{m'}\rangle C_{n,m'}^{(p-1)} - \sum_{j=1}^{p} E_n^{(j)} C_{n,m}^{(p-j)}\right). \tag{11}$$

Together with $C_{n,m}^{(0)} = \delta_{n,m}$ and $E_n^{(0)} = \epsilon_n$ these relations form a recursive set of equations which uniquely determines the perturbative corrections for all energies and states to all orders.

Usually one would use these general expressions to derive explicit formulae for the lowest-order corrections. The matrix elements of the perturbation in the unperturbed Slater-determinant states can be evaluated explicitly and the summations over the many-body basis set can be replaced by summations over single-particle states. In this way we would recover the standard expressions for, e.g., the second- and third-order energy corrections [8,11,16].

2.2. Evaluation to high orders

When attempting to evaluate the perturbative corrections beyond third- or forth-order the explicit formulae for the energy corrections become impractical because of the large number of nested summations. A much more elegant way to evaluate high-order contributions makes use of the recursive structure of Eqs. (10) and (11). The only ingredients needed are the many-body matrix elements of the full Hamiltonian H with respect to the unperturbed basis $|\Phi_n\rangle$. Starting from the zeroth-order coefficients $C_{n,m}^{(0)} = \delta_{n,m}$ we can readily evaluate the first-order energy contribution $E_n^{(1)}$ from (10). This in turn allows us to compute the first-order coefficients $C_{n,m}^{(1)}$ via (11). Generally, for the evaluation of the energy contribution $E_n^{(p)}$ only the coefficients $C_{n,m}^{(p-1)}$ of the previous order are required. For the evaluation of the coefficients $C_{n,m}^{(p)}$ all energy contributions up to order p and all coefficients up to order $(p-1)$ need to be known.

Technically, the recursive evaluation of the perturbation series bears some resemblance to the Lanczos algorithm for the iterative solution of the eigenvalue problem for a few extremal eigenvalues as it is used in the NCSM. The most significant operation is a matrix-vector multiplication of the Hamiltonian matrix with the coefficient vector from the previous order, which constitutes the first term in the evaluation of the coefficients (11). Because the second term in (11) involves the coefficient vectors from all previous orders, we store them for simplicity. These computational elements are the same as for a simple Lanczos algorithm