Bachelor-Thesis

Many-Body Perturbation Theory for the Nuclear Many-Body Problem



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August - October 2006

Working within the framework of the Unitary Correlation Operator Method (UCOM), this work presents the derivation of an exact-denominator version of the second-order many-body perturbation theory correction to the Hartree-Fock ground state energy. In addition, corrections to the Hartree-Fock single-particle energies are investigated.

Contents

Contents

1.	Introduction						
2.	Calculating Ground-State Energies with UCOM-HF 2.1. Unitary Correlation Operator Method (UCOM)	4 5 6 9					
3.	Many-Body Perturbation Theory (MBPT)3.1. Rayleigh-Schrödinger (RS) MBPT3.2. Brillouin-Wigner (BW) MBPT	10 10 13					
4.	Improved MBPT Calculations4.1. Exact Denominator (ED) of Second-Order MBPT4.2. Calculations done with ED4.3. Evaluation and Interpretation of the Results	14 14 15 15					
5.	Corrections for Single-Particle (SP) Energies5.1. Estimating Single-Particle Energies5.2. Calculations and Results of SP Energy Corrections	19 19 22					
6.	o. Outlook 22						
Α.	A. Slater rules 24						
B.	3. Brief Description of BW MBPT 26						
C.	C. Implementation-specific Remarks C.1. Changes to nsuite						
D.	D. Additional Graphs 28						

1. Introduction

1. Introduction

The description of ground-state properties of heavier nuclei based on realistic nucleonnucleon (NN) interactions, reproducing the experimental NN scattering data, is still an unsolved problem in the theory of nuclear structure. In state-of-the-art calculations light nuclei can be described in *ab initio*¹ schemes like the no-core shell model or Green's function Monte Carlo. However, these methods are currently computationally too expensive to be applied to heavier nuclei.

Approximating many-body states in managable model spaces of simple antisymmetric Slater determinants one encounters two properties of realistic NN interactions which lead to difficulties. Those are (i) a strong short-ranged (< 0.5 fm) repulsion and (ii) a strong tensor force. These interaction components cause high momenta which are associated with states not included in a space spanned by a small number of Slater determinants. Huge Hilbert spaces would be needed to describe such states to a reasonable degree.

We perform a unitary transformation of the bare realistic NN interaction to make the many-body problem tractable with model spaces and methods which can be employed over the whole nuclear chart. This unitary transformation explicitly describes the short-range central and tensor correlations induced by the NN interaction, and is the key idea of the Unitary Correlation Operator Method (UCOM).

In our calculations we start with a Hamiltonian transformed by UCOM. First, a standard Hartree-Fock (HF) scheme is applied. Further, we apply many-body perturbation theory (MBPT) to the HF solution in order to introduce residual long-range correlations. A summary of the essential steps is given in Sec. 2 and 3.

The aim of this work is to improve the MBPT calculations. To simplify the formula of the MBPT correction of the energy, an approximation was made in previous calculations: the second-order term was calculated with a simplified denominator. In Sec. 4 we undo this step and calculate a more precise energy correction of MBPT. This section also includes a discussion of the deviation of the obtained results from former ones. Furthermore, we employ MBPT as a tool to calculate corrections to the single-particle (SP) energies in Sec. 5.

2. Calculating Ground-State Energies with UCOM-HF

Since bare realistic potentials, like the Argonne V18 (AV18) potential, are unsuitable for simple many-body model spaces that single Slater determinants provide, they must be modified to yield reasonable results. The Unitary Correlated Operator Method (UCOM) provides a novel approach to describe short-range central and tensor correlations explicitly by a unitary transformation. Since the correlation operators are given explicitly, UCOM allows for the derivation of a basis-independent effective interaction operator $V_{\rm UCOM}$. To compute ground-state energies of nuclei, the HF scheme is employed.

In the present treatment of the nuclear many-body problem, we restrict ourselves to two-body interactions, not considering higher orders of the *cluster expansion* of corre-

¹I.e., without introducing approximations to the nuclear many-body problem with realistic interactions.

lated operators (cf. Sec. 2.2). This approximation seems reasonable supposing that the range of the correlations is short compared to the mean particle distances. A brief discussion of UCOM is presented in this section. For more details refer to [1, 2, 3, 4].

2.1. Unitary Correlation Operator Method (UCOM)

For computational reasons many-body states are preferentially approximated by single antisymmetric² Slater determinants

$$\left|\Psi\right\rangle_{a} = \mathcal{A}\left(\left|\alpha_{1}\right\rangle \otimes \left|\alpha_{2}\right\rangle \otimes \ldots \otimes \left|\alpha_{A}\right\rangle\right) , \qquad (2.1)$$

where

$$\left|\alpha_{i}\right\rangle = \left|\varphi_{i}\right\rangle \otimes \left|\chi_{i}\right\rangle \otimes \left|\tau_{i}\right\rangle$$

is a single-particle (SP) state with spatial component $|\varphi_i\rangle$, spin component $|\chi_i\rangle$ and isospin component $|\tau_i\rangle$.

The UCOM transforms the critical central and tensor parts of the realistic interaction by a *correlation operator* C, conserving inherent operator symmetries and the NN phase shifts. This *correlation operator* C can be written as the product of two independent unitary operators describing the tensor and the central correlations, respectively:

$$C = C_{\Omega}C_{r} = \exp\left[-i\sum_{i< j} g_{\Omega,ij}\right] \exp\left[-i\sum_{i< j} g_{r,ij}\right]$$
(2.2)

The hermitian two-body generators g_r and g_{Ω} are given by

$$g_r = \sum_{S,T} \frac{1}{2} \left[s_{ST}(r) q_r + q_r s_{ST}(r) \right] \Pi_{ST}$$
(2.3)

$$g_{\Omega} = \sum_{T} \vartheta_{T}(r) s_{12}(\mathbf{r}, \mathbf{q}_{\Omega}) \Pi_{1T} , \qquad (2.4)$$

where relative momentum \mathbf{q} , relative distance operator \mathbf{r} , radial momentum q_r , orbital momentum \mathbf{q}_{Ω} , and $s_{12}(\mathbf{r}, \mathbf{q}_{\Omega})$ are defined by the following relations:

$$\mathbf{q} = \frac{1}{2} \left[\mathbf{p}_1 - \mathbf{p}_2 \right] , \ \mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2 , \ q_r = \frac{1}{2} \left[\frac{\mathbf{r}}{r} \cdot \mathbf{q} + \mathbf{q} \cdot \frac{\mathbf{r}}{r} \right]$$
(2.5)

$$\mathbf{q}_{\Omega} = \mathbf{q} - \frac{\mathbf{r}}{r} q_r = \frac{1}{2r^2} \left[\mathbf{l} \times \mathbf{r} - \mathbf{r} \times \mathbf{l} \right]$$
(2.6)

$$s_{12}(\mathbf{r}, \mathbf{q}_{\Omega}) = \frac{3}{2} \left[(\boldsymbol{\sigma}_1 \cdot \mathbf{q}_{\Omega}) (\boldsymbol{\sigma}_2 \cdot \mathbf{r}) - (\boldsymbol{\sigma}_2 \cdot \mathbf{r}) (\boldsymbol{\sigma}_1 \cdot \mathbf{q}_{\Omega}) \right] .$$
(2.7)

 \mathbf{x}_i and \mathbf{p}_i denote the particle position and momentum, \mathbf{l} is the orbital angular momentum, and σ_i are the spin operators.

 $^{^{2}}$ The index *a* for antisymmetric states is omitted in the following for the sake of brevity. All states are assumed to be antisymmetric.

The central correlator C_r shifts a pair of particles apart by a distance-dependent amount in the radial direction, until they are out of the range of the repulsive core. $s_{ST}(r)$ is the shift as a function of the inter-particle distance for each spin-isospin channel.

The tensor correlator C_{Ω} does not act in the S = 0 channels. The impact of the tensor correlator C_{Ω} in the S = 1 channels is a perpendicular shift to the relative orientation **r**. $\vartheta_T(r)$ describes strength and range of the tensor correlations. It is only a function of the inter-particle distance. Both $s_{ST}(r)$ and $\vartheta_T(r)$ vanish for large distances, and the correlators reduce to identity operators.

The optimal correlation functions are determined variationally for each (S,T)-channel by minimizing the energy of the two-nucleon system. The correlation volume

$$I_{\vartheta} = \int \mathrm{d}r \cdot r^2 \vartheta(r) \tag{2.8}$$

imposes an additional constraint on the range of the tensor correlation. More details can be obtained from [4] and [5].

As an example, Fig. 1 panel (a) depicts a radial two-body wave function as it typically results from a single Slater determinant. Note the high, unrealistic probability at small interparticle distances ($r < 1 \,\mathrm{fm}$). This flaw is eliminated by application of the *central correlator*³ c_r to the state, in panel (c). Panel (e) shows the consequences of the application of the *tensor correlator* c_{Ω} to a radial s-wave two-body wave function. In panels (b), and (d) of Fig. 1 the central and tensor correlation functions are displayed schematically.

Fig. 2 visualizes how the troublesome higher off-diagonal matrix elements in relative momentum-space (of the form $\langle q(LS)JT | v_{\text{UCOM}} | q'(L'S)JT \rangle$, where q is the relative two-body momentum) are moved closer to the zero-plane by the unitary transformation. The low-momentum matrix elements become strongly attractive. The inclusion of the *tensor correlator* does not change the matrix elements of the spin-singlet channel, but suppresses off-diagonal matrix elements in the spin-triplet channel. Thus, the unitary transformations "prediagonalizes" the interaction, decoupling low and high momenta.

2.2. Correlated Interaction V_{UCOM}

Now we will apply the *correlation operator* C to an uncorrelated Hamiltonian and calculate correlated matrix elements of the effective correlated potential V_{UCOM} .

To distinguish correlated and uncorrelated operators and states, correlated operators and states are denoted by a tilde, i.e. $|\tilde{\Psi}\rangle = C |\Psi\rangle$ for a correlated many-body state and $\tilde{A} = C^{\dagger}AC$ for a correlated operator.

A transformation of an arbitrary operator A leads to a correlated operator with contributions to all particle numbers. We formulate a *cluster expansion* [1] of the correlated operator

$$\widetilde{\mathbf{A}} = \widetilde{\mathbf{A}}^{[1]} + \widetilde{\mathbf{A}}^{[2]} + \widetilde{\mathbf{A}}^{[3]} + \dots , \qquad (2.9)$$

³Small letters denote two-body operators.



Figure 1: Application of the central and tensor correlators resulting in a transformed s-wave two-body trial state, as onbtained from the Argonne V18 potential. Panels (a), (c) and (e) depict the uncorrelated, the central correlated, and the central and tensor correlated radial wave function, respectively. The panels (b) and (d) show the corresponding central and tensor correlation functions, where $R_{\pm}(r) \approx r \pm s(r)$ for slowly varying shift functions s(r). $I_{\vartheta} = 0.09 \,\mathrm{fm}^3$.

where the irreducible *n*-body contributions are denoted by $\widetilde{A}^{[n]}$. When starting with a *k*-body operator irreducible contributions with n < k vanish.

Consider an uncorrelated Hamiltonian H consisting of an one-body kinetic energy $T = \sum_i \mathbf{p}_i^2/(2m_N)$ and a two-body interaction $V = \sum_{i < j} v_{ij}$. As long as the range of the correlation functions s(r) and $\vartheta(r)$ is small compared to mean particle distances, the higher particle number contributions of the cluster expansion of the correlated Hamiltonian \widetilde{H} are negligible. This leads us to the following two-body approximation⁴:

$$\widetilde{\mathbf{H}}^{C2} = \widetilde{\mathbf{T}}^{[1]} + \widetilde{\mathbf{T}}^{[2]} + \widetilde{\mathbf{V}}^{[2]} \equiv \mathbf{T} + \mathbf{V}_{\text{UCOM}} , \qquad (2.10)$$

where $\widetilde{T}^{[1]}$ turns out to be the simple uncorrelated kinetic energy. The two-body terms are subsumed in a correlated effective interaction $V_{\text{UCOM}} = \sum_{i < j} v_{\text{UCOM},ij}$. V_{UCOM} can be considered a realistic potential on its own. The fact that an explicit form of the correlated operator exists makes it applicable in methods which do not allow the use of partial wave matrix elements.

To apply the correlated interaction V_{UCOM} in a HF scheme formulated in the spherical harmonic-oscillator basis we have to calculate its two-body matrix elements. We employ jj-coupled harmonic-oscillator states $|n_1l_1j_1, n_2l_2j_2; JT\rangle$ for this purpose. It turns out

⁴The two-body approximation is denoted by the superscript C2.



Figure 2: Relative momentum-space matrix elements $\langle q(LS)JT | v_{\text{UCOM}} | q'(L'S)JT \rangle$ of the bare AV18 potential (left-hand column), the central-correlated AV18 potential (center column), and the fully correlated AV18 potential. The different rows correspond to different partial waves, as indicated on the left-hand side. The red dots mark the plane of vanishing matrix elements. The momenta are given in fm⁻¹ and the matrix elements in MeV.

that it is computationally more effective to map the *tensor correlator* C_{Ω} back onto the two-body states whereas the *central correlator* C_r acts onto the operators. Skipping the extensive derivation [5, 7, 9], the non-normalized antisymmetric *jj*-coupled matrix elements read as follows:

$$\left\langle n_{1}l_{1}j_{1}, n_{2}l_{2}j_{2}; JT \right| \operatorname{v}_{\mathrm{UCOM}} \left| n_{1}'l_{1}'j_{1}', n_{2}'l_{2}'j_{2}'; JT \right\rangle =$$

$$= \sqrt{[j_{1}][j_{2}][j_{1}'][j_{2}']} \sum_{L,L',S} \sum_{N,\Lambda} \sum_{\nu,\lambda} \sum_{\nu',\lambda'} \sum_{j} \left\{ \begin{array}{cc} l_{1} & l_{2} & L \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{1} & j_{2} & J \end{array} \right\} \cdot$$

$$\cdot \left\{ \begin{array}{cc} l_{1}' & l_{2}' & L' \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{1}' & j_{2}' & J \end{array} \right\} \left\{ \begin{array}{cc} \Lambda & \lambda & L \\ S & J & j \end{array} \right\} \left\{ \begin{array}{cc} \Lambda & \lambda' & L' \\ S & J & j \end{array} \right\} \cdot$$

$$\cdot \left\langle \langle N\Lambda, \nu\lambda | n_{1}l_{1}, n_{2}l_{2}; L \rangle \rangle \left\langle \langle N\Lambda, \nu'\lambda' | n_{1}'l_{1}', n_{2}'l_{2}'; L' \rangle \right\rangle \cdot$$

$$\cdot [j] [S] [L] [L'] (-1)^{L+L'} \left\{ 1 - (-1)^{\lambda+S+T} \right\} \cdot$$

$$\cdot \left\langle \nu(\lambda S)jT | \operatorname{v}_{\mathrm{UCOM}} | \nu'(\lambda'S)jT \right\rangle .$$

$$(2.11)$$

 $n, n' = 0, 1, 2, \ldots$ are the radial oscillator quantum numbers, $[j] \equiv 2j + 1$, and $\{\ldots\}$ are the 6j and 9j symbols. Moreover, $\langle \langle \ldots | \ldots \rangle \rangle$ are the harmonic oscillator brackets [12, 13].

2.3. UCOM applied to a Hatree-Fock (HF) Scheme

The standard HF scheme is a variational approach to the nuclear many-body problem. It assumes an A-body state as in Eq. 2.1. The $|\alpha_i\rangle$ are the variational degrees of freedom used to minimize the expectation value of the Hamiltonian. The variational solution of the many-body states then leads to the HF equations [11].

The Hamiltonian consists in our case of the effective realistic potential V_{UCOM} and the intrinsic kinetic energy T_{int} :

$$H_{int} = T_{int} + V_{UCOM} . \qquad (2.12)$$

Center-of-mass contributions are excluded from the energy, i.e. the center-of-mass kinetic energy T_{cm} is subtracted from the kinetic energy to yield the intrinsic kinetic energy:

$$T_{\rm int} = T - T_{\rm cm} = \frac{2}{A} \frac{1}{m_N} \sum_{i < j}^{A} \mathbf{q}_{ij}^2 . \qquad (2.13)$$

It depends only on the relative two-body momentum \mathbf{q}_{ij} . This leads to a Hamiltonian \mathbf{H}_{int} which is Galilei-invariant and a quasi two-body operator. The effect of center-of-mass excitations to \mathbf{T}_{int} is not excluded, however, it is expected to yield only a small contribution.

The jj-coupled Hartree-Fock SP states $|a\rangle$ expressed in the harmonic oscillator basis read

$$\left|a\right\rangle = \left|\nu(l\frac{1}{2})jm; \frac{1}{2}m_t\right\rangle \equiv \left|\nu ljmm_t\right\rangle = \sum_n C_n^{(\nu ljmm_t)} \left|n ljmm_t\right\rangle,$$
(2.14)



Figure 3: Binding energies resulting from a HF calculation with a correlated AV18 ($I_{\vartheta} = 0.09 \text{ fm}^3$), (\bigcirc) in reference to the experimental values (\longrightarrow). HF calculations were done for $e_{\text{Max}} = 12$, $l_{\text{Max}} = 10$.

with radial harmonic-oscillator quantum number n, orbital angular momentum l, total angular momentum j with projection m, and isospin projection m_t .

The regular iterative HF scheme enables us to calculate the HF energies [4]. To do so we use a truncated harmonic oscillator basis with $e = 2n + l \le e_{\text{Max}}$ and optionally $l \le l_{\text{Max}}$.

Using this HF framework with a correlated AV18 potential we obtain the binding energies shown in Fig. 3. Although a sizable (nearly constant!) difference to experimental results remains, we are able to obtain bound states, which would be impossible with a bare interaction.

The primal cause of the deviation to experimental results are the binding energy contributions from long-range correlations, which are not covered by the UCOM-HF scheme. Assessing these neglected correlations is the subject of the next section.

3. Many-Body Perturbation Theory (MBPT)

To account for the effect of the residual long-range correlations the HF solution is corrected by MBPT [10]. More precisely, we add the first non-vanishing order of MBPT, which is the second-order, to the HF energies.

3.1. Rayleigh-Schrödinger (RS) MBPT

Rayleigh-Schrödinger (RS) MBPT is the simplest and most frequently used form of MBPT.

The original Hamiltonian H is divided into an unperturbed Hamiltonian H₀ and a perturbative Hamiltonian W, related by $H = H_0 + \lambda W$, with $0 \le \lambda \le 1$. λ is a formal expansion parameter and will be set later to unity. Next, the exact eigenfunctions and eigenvalues of the corresponding Schrödinger equation are expanded in a series in λ ,

$$E_i = E_i^{(0)} + \lambda E_i^{(1)} + \lambda^2 E_i^{(2)} + \dots$$
(3.1)

$$\left|\Phi_{i}\right\rangle = \left|\Phi_{i}^{(0)}\right\rangle + \lambda \left|\Phi_{i}^{(1)}\right\rangle + \lambda^{2} \left|\Phi_{i}^{(2)}\right\rangle + \dots \qquad (3.2)$$

We assume the unperturbed wavefunction to be normalized, $\langle \Phi_i^{(0)} | \Phi_i^{(0)} \rangle = 1$, and choose a beneficial *intermediate* normalization, $\langle \Phi_i | \Phi_i^{(0)} \rangle = 1$, for $| \Phi_i \rangle$. In consequence, we find $\langle \Phi_i | \Phi_i^{(n)} \rangle = 0$ for n = 1, 2, 3, ...

Eqs. 3.1 and 3.2 are related by the Schrödinger equation. Comparing λ -coefficients one easily obtains following set of relations:

$$H_0 |\Phi_i^{(0)}\rangle = E_i^{(0)} |\Phi_i^{(0)}\rangle$$
(3.3)

$$H_{0} \left| \Phi_{i}^{(1)} \right\rangle + W \left| \Phi_{i}^{(0)} \right\rangle = E_{i}^{(0)} \left| \Phi_{i}^{(1)} \right\rangle + E_{i}^{(0)} \left| \Phi_{i}^{(0)} \right\rangle$$

$$(3.4)$$

$$H_{0} |\Phi_{i}^{(2)}\rangle + W |\Phi_{i}^{(1)}\rangle = E_{i}^{(0)} |\Phi_{i}^{(2)}\rangle + E_{i}^{(1)} |\Phi_{i}^{(1)}\rangle + E_{i}^{(2)} |\Phi_{i}^{(0)}\rangle$$

$$H_{0} |\Phi_{i}^{(3)}\rangle + W |\Phi_{i}^{(2)}\rangle = E_{i}^{(0)} |\Phi_{i}^{(3)}\rangle + E_{i}^{(1)} |\Phi_{i}^{(2)}\rangle +$$

$$(3.5)$$

$$+ E_{i}^{(2)} \left| \Phi_{i}^{(1)} \right\rangle + E_{i}^{(3)} \left| \Phi_{i}^{(0)} \right\rangle .$$
(3.6)

Upon combining these equations they lead to the following expressions for the nth-order energies:

$$E_{i}^{(0)} = \left\langle \Phi_{i}^{(0)} \middle| \mathbf{H}_{0} \middle| \Phi_{i}^{(0)} \right\rangle$$
(3.7)

$$E_i^{(1)} = \left\langle \Phi_i^{(0)} \middle| W \middle| \Phi_i^{(0)} \right\rangle$$
(3.8)

$$E_i^{(2)} = \left\langle \Phi_i^{(0)} \middle| W \middle| \Phi_i^{(1)} \right\rangle$$
(3.9)

$$E_i^{(3)} = \left\langle \Phi_i^{(0)} \middle| W \middle| \Phi_i^{(2)} \right\rangle$$

$$E_i^{(4)} = \dots$$
(3.10)

Solving again the set of Eqs. 3.3 – 3.6, this time for $|\Phi_i^{(k)}\rangle$ one can determine the *k*thorder energy with Eqs. 3.7 – 3.10. We write $|\Phi_i^{(1)}\rangle$ inserting the unity operator in form of the H₀ eigenstates $|n\rangle \equiv |\Phi_n^{(0)}\rangle$:

$$\left|\Phi_{i}^{(1)}\right\rangle = \sum_{n} \left|n\right\rangle \left\langle n\right|\Phi_{i}^{(1)}\right\rangle = \sum_{n\neq i} \left|n\right\rangle \left\langle n\right|\Phi_{i}^{(1)}\right\rangle, \qquad (3.11)$$

where the last representation is obtained due to the *intermediate* normalization. $\langle n | \Phi_i^{(1)} \rangle$ is zero for i = n. Multiplying Eq. 3.4 by $\langle n |$, one finds

$$(E_i^{(0)} - E_n^{(0)}) \langle n | \Phi_i^{(1)} \rangle = \langle n | W | \Phi_i^{(0)} \rangle, \qquad (3.12)$$

considering that the zeroth-order wave functions are orthogonal.

Now we substitute the expansion Eq. 3.11 into Eq. 3.9:

$$E_i^{(2)} = \left\langle \Phi_i^{(0)} \middle| W \middle| \Phi_i^{(1)} \right\rangle = \sum_{n \neq i} \left\langle \Phi_i^{(0)} \middle| W \middle| n \right\rangle \left\langle n \middle| \Phi_i^{(1)} \right\rangle, \qquad (3.13)$$

and finally, upon combining this equation with Eq. 3.12 the expression for the secondorder energy

$$E_i^{(2)} = \sum_{n \neq i} \frac{\left| \langle i | \mathbf{W} | n \rangle \right|^2}{E_i^{(0)} - E_n^{(0)}}$$
(3.14)

3. Many-Body Perturbation Theory (MBPT)

can be written in terms of the solutions of the initial unperturbed eigenproblem.

Likewise, expressions for higher order energies and states can be obtained. It is also possible to calculate higher order energies iteratively.

In our case the eigenbasis $|n\rangle$ consists of the eigenstates of the HF solution. The unperturbed Hamiltonian is associated with the diagonal matrix elements of H_{int}. In second quantization its two-body part reads

$$\mathbf{H}_{0} = \sum_{\alpha\beta} \left\langle \left. \alpha\beta \right| \mathbf{H}_{\text{int}} \left| \alpha\beta \right. \right\rangle \mathbf{a}_{\alpha}^{\dagger} \mathbf{a}_{\beta}^{\dagger} \mathbf{a}_{\beta} \mathbf{a}_{\alpha} \,, \qquad (3.15)$$

where a^{\dagger} is the creation operator and a the extinction operator. The perturbation W consists of the off-diagonal contributions of the correlated Hamiltonian $\langle \alpha\beta | H_{int} | \delta\gamma \rangle$ with $\alpha \neq \delta$, $\beta \neq \gamma$, $\alpha \neq \gamma$, or $\beta \neq \delta$.

To describe excited Slater determinants, we introduce the following conventions: the latin letters a, b, c, \ldots are used to denote occupied one-particle states below the Fermi energy ϵ_F (hole states). The letters r, s, t, \ldots mark states above Fermi energy ϵ_F (particle states). Further, latin subscripts following a many-body state or energy denote removed particles, whereas superscripts indicate newly occupied states. For instance, the many-body state $|\Psi_{ab}^{rs}\rangle$ denotes a state where originally all levels beneath the Fermi energy were occupied. The indices following Ψ tell us that the particles of the levels a, b were removed whereas the levels r, s were newly occupied. Similarly, E_{ab}^{rs} is shorthand for $\langle \Psi_{ab}^{rs} | \operatorname{H_{int}} | \Psi_{ab}^{rs} \rangle$.

Originally, the sum in Eq. 3.14 runs over all possible excitations $|n\rangle$. Yet, we can exclude certain excitations types when applying it to our framework. Single-excitation HF Slater determinants are absent in the sum because of Brillouin's theorem⁵, while triple and higher order determinants do not appear because the Hamiltonian contains at most two-particle interactions. Hence, the second-order perturbation theory deals with a correction induced by the subspace of 2p2h-states⁶ ($|\Psi_{ab}^{rs}\rangle$).

We find for the ground state energy correction following Eq. 3.14:

$$E_0^{(2)} \equiv E^{(2)} = \sum_a \sum_{b < a} \sum_r \sum_{s < r} \frac{\left| \left\langle \Psi_0 \right| \operatorname{H}_{\operatorname{int}} \left| \Psi_{ab}^{rs} \right\rangle \right|^2}{E^{(0)} - E_{ab}^{rs}} \,. \tag{3.16}$$

Using the Slater rules (App. A) we rewrite the numerator,

$$E^{(2)} = \frac{1}{4} \sum_{a,b} \sum_{r,s} \frac{\left| \langle ab | \operatorname{H}_{\operatorname{int}} | rs \rangle \right|^2}{E^{(0)} - E^{rs}_{ab}} .$$
(3.17)

To make this approach computationally less demanding an additional approximation was used in the previous calculations [4]:

$$E^{(0)} - E^{rs}_{ab} = \left\langle \Psi^{rs}_{ab} \right| E^{(0)} - \mathcal{H}_{int} \left| \Psi^{rs}_{ab} \right\rangle \cong \epsilon_a + \epsilon_b - \epsilon_r - \epsilon_s , \qquad (3.18)$$

⁵Brillouin's theorem states that the HF equations can be rewritten as a decoupling condition between ground-state and one-particle-one-hole (1p1h) excitations.

 $^{^6\}mathrm{Shorthand}$ for two-partice-two-hole-states.



Figure 4: Binding energies resulting from HF+MBPT calculations (\bigcirc), where UCOM was applied to the Hamiltonian initially, in reference to the experimental values (—). HF calculations were done with $e_{\text{Max}} = 12$, $l_{\text{Max}} = 10$ (AV 18, $I_{\vartheta} = 0.09 \text{ fm}^3$).

where ϵ_x are the HF SP energies of the corresponding states.

Employing the expressions given above, the ground state energies for selected closedshell nuclei were calculated in Ref. [4]. These calculations use a correlated AV18 potential, a correlation volume $I_{\vartheta} = 0.09$ fm and 13 major oscillator shells ($e_{\text{Max}} = 12$, $l_{\text{Max}} = 10$). It is found that the resulting energies reproduce the experimental data to a good extent throughout the nuclear chart from ⁴He to ²⁰⁸Pb and even far off the valley of β -stability (Fig. 4). In order to estimate higher order perturbative effects, the third order was also calculated but yielded only a small deviation from second-order results, indicating a possible onset of convergence of the perturbation series. The suprisingly good results for the binding energies in two-body approximation are accredited to a net cancellation of three-body effects [14].

However, theoretical results obtained from no-core shell model⁷ calculations indicate that some additional binding energy can still be gained from long-range correlations.

3.2. Brillouin-Wigner (BW) MBPT

Another variant of MBPT is the Brillouin-Wigner (BW) scheme. This method yields often better results, at the same order of MBPT than Rayleigh-Schröder (RS) MBPT. Moreover, it is often an easy way to avoid the somewhat demanding case of degenerated RS MBPT, given that the degeneracies are resolved in the aspired order of MBPT.

Contrary to the RS MBPT, the BW MBPT already uses the final energy in the definition of the energy contribution and so requires an iterative scheme for the calculation. For a compact description, see App. B.

⁷The no-core shell model provides the "exact" solution of the many-body problem for a given interaction, i.e. long-range correlations are fully included (Ref. [5]).

4. Improved MBPT Calculations

In the last section MBPT was used to assess the impact of residual long-ranged correlations not treated by the HF method. To be more accurate in our calculation, we will undo the approximation made in Eq. 3.18 and calculate MBPT with an exact denominator (ED). Afterwards we evaluate the changes in the obtained results.

BW MBPT is not further considered. First, as it is computationally very demanding. (It requires an iterative scheme, and net energy cancellations, which reduce the denominator-sum in RS MBPT extremely, do not occur in the BW variant.) Furtheron, the deviation from results obtained from RS MBPT calculations is expected to be small.

As the following methods were newly implemented we will address possible complications in the course of the discussion, and will also make some programmcode-specific comments.

4.1. Exact Denominator (ED) of Second-Order MBPT

Let us go back to Eq. 3.17 and manipulate the denominator:

$$E^{(0)} - E^{rs}_{ab} = \left\langle \Psi_0 \right| \operatorname{H}_{\operatorname{int}} \left| \Psi_0 \right\rangle - \left\langle \Psi^{rs}_{ab} \right| \operatorname{H}_{\operatorname{int}} \left| \Psi^{rs}_{ab} \right\rangle .$$

$$(4.1)$$

Applying the Slater rules and considering the cancellation of matrix elements not including either a,b or r,s one obtains:

$$\left\langle \Psi_{0} \middle| \operatorname{H}_{\operatorname{int}} \middle| \Psi_{0} \right\rangle - \left\langle \Psi_{ab}^{rs} \middle| \operatorname{H}_{\operatorname{int}} \middle| \Psi_{ab}^{rs} \right\rangle =$$

$$= \frac{1}{2} \left\{ \sum_{d,e} \left\langle de \middle| \operatorname{H}_{\operatorname{int}} \middle| de \right\rangle - \sum_{d,e} \left\langle de \middle| \operatorname{H}_{\operatorname{int}} \middle| de \right\rangle \right\} =$$

$$= \sum_{d} \left\langle ad \middle| \operatorname{H}_{\operatorname{int}} \middle| ad \right\rangle + \sum_{d}^{d \neq a} \left\langle bd \middle| \operatorname{H}_{\operatorname{int}} \middle| bd \right\rangle -$$

$$- \sum_{d} \left\langle rd \middle| \operatorname{H}_{\operatorname{int}} \middle| rd \right\rangle - \sum_{d}^{d \neq r} \left\langle sd \middle| \operatorname{H}_{\operatorname{int}} \middle| sd \right\rangle,$$

$$(4.2)$$

where prime 'indicates that in the summation over the occupied SP states the following replacement is made: $a \to r$ and $b \to s$. This simplified denominator is then used for further calculations.

First, the ED MBPT was implemented in the *standard* calculation method (HFM) which consists in adding explicitly the energy contributions of all SP levels. It turned out that calculations done with this method were extremely time-consuming and only the ground state energies of lighter nuclei could be obtained in a reasonable time. To make the routine more efficient, we restricted the calculations to closed-shell nuclei, benefitting from averaging over the contributions due to different *m*-values (HFC) and thereby reducing the sums in Eq. 3.17.⁸ For closed shells the HFC method is "exact"

⁸The calculation time for ⁹⁰Zr with $e_{\text{Max}} = 12$, $l_{\text{Max}} = 10$ is ~ 10 d.

Nucleus	⁴ He	$^{16}\mathrm{O}$	^{24}O	$^{34}\mathrm{Si}$	$^{40}\mathrm{Ca}$	$^{48}\mathrm{Ca}$	$^{48}\mathrm{Ni}$	56 Ni	$^{78}\mathrm{Ni}$	$^{88}\mathrm{Sr}$	$^{90}\mathrm{Zr}$
$a_{\rm HO}({\rm fm})$	1.3	1.5	1.7	1.6	1.6	1.7	1.7	1.7	1.8	1.8	1.8

Table 1: Optimal Oscillator Length for selected closed-shell Nuclei.

Nucleus	⁴ He	$^{16}\mathrm{O}$	$^{24}\mathrm{O}$	$^{34}\mathrm{Si}$	$^{40}\mathrm{Ca}$	$^{48}\mathrm{Ca}$	$^{48}\mathrm{Ni}$	56 Ni	$^{78}\mathrm{Ni}$	$^{88}\mathrm{Sr}$	$^{90}\mathrm{Zr}$
$\Delta E(\text{MeV})$	4.24	5.84	2.75	5.69	6.08	-3.26	-2.43	-3.69	4.72	5.08	5.07

Table 2: Deviation of the results of ED MBPT from AD MBPT for selected closed-shell nuclei, calculated with HFC and $e_{\text{Max}} = 12$, $l_{\text{Max}} = 10$.

- within the framework of HF calculations, but it constitutes an approximation for the energy contributions from shells containing the two-hole states and the shells containing the two excited nucleons above Fermi energy.

4.2. Calculations done with ED

The calculations made with the exact-denominator (ED) method were restricted to some selected representative closed-shell nuclei used in previous calculations: ⁴He, ¹⁶O, ²⁴O, ³⁴Si, ⁴⁰Ca, ⁴⁸Ca, ⁴⁸Ni, ⁵⁶Ni, ⁷⁸Ni, ⁸⁸Sr, ⁹⁰Zr.

A correlated AV18 potential and a correlation volume of $I_{\vartheta} = 0.09 \text{ fm}^3$ were used for the calculations in both the HFM and the HFC method. In a first HF run, the optimal oscillator lengths a_{HO} were determined for each nucleus (cf. Tab. 1).

Employing the HFM method, two runs were done: The first one with a basis of 11 major oscillator shells ($e_{\text{Max}} = 10$). This configuration allowed us only to calculate some lighter nuclei. The second one with a smaller basis of $e_{\text{Max}} = 8$ and therefore a shorter calculation time. With the HFC method we performed calculations for each $e_{\text{Max}} = 6, 8, 10$, and $e_{\text{Max}} = 12$ with the additional restriction $l_{\text{Max}} = 10$. Similar calculations with the approximated-denominator (AD) method were done for comparison.

4.3. Evaluation and Interpretation of the Results

The newly calculated ED MBPT energy corrections give mostly a little lower binding energies than the AD MBPT calculations. Fig. 5 depicts the binding energies calculated with the old AD MBPT vs. the ones calculated with HFC ED MBPT.

Fig. 6 also displays values for the binding energies obtained by treating the longranged correlations by means of random phase approximation (RPA) [8]. The values of the ED variant are usually closer to the RPA results. The mean deviation between the AD method and the ED method is $\Delta \bar{E} = 4.4 \text{ MeV}$ (cf. Tab. 2).

Employing a realistic NN potential for the description of nuclear ground states, sets a theoretical framework for the calculations which does not describe perfectly the physical circumstances – hence, even an exact solution of the many-body problem within this interaction might yield a deviation from the experimental results. Two binding energies



Figure 5: Binding energies for representative closed-shell nuclei, resulting from HF-scheme+AD MBPT calculations (●) vs. HF-scheme+ED MBPT calculations (■). Furthermore, experimental values (—) are displayed. HF and MBPT calculations were done with the HFC code and e_{Max} = 12 with restriction l_{Max} = 10.



Figure 6: Binding energies for some representative closed-shell nuclei: AD MBPT (\bigcirc), ED MBPT (\blacksquare), RPA (\blacklozenge), experimental values (\longrightarrow), and exact values within theoretical framework (\blacktriangle) of ⁴He and ¹⁶O originating from the no-core shell model. MBPT and HF calculations were done with the HFC code and $e_{\text{Max}} = 12$ with restriction $l_{\text{Max}} = 10$.



Figure 7: Comparison of the two MBPT calculations methods, HFM (\bigcirc) and HFC (\blacksquare). MBPT calculations were done with $e_{\text{Max}} = 8$.

calculated by applying the no-core shell model with a realistic NN potential are displayed in Fig. 6. These energy values are exact within our framework given by $V_{\rm UCOM}$.

As a result of the method-intrinsic deviation discussed above, experimental values⁹ can only give us a messure for the overall quality of the many-body approximation, but they make it difficult to differentiate between the quality of distinct approximation methods within the accuracy level reached by these approximations. Exact values within our theoretical framework can presently only be calculated for low-mass nuclei. Those values hint at somewhat lower binding energies than the experimental binding energies (Ref. [5, 6]).

There is a deviation of the ground state energies obtained from the HFC method to those obtained from the exact HFM method, but Fig. 7 shows that the approximation is quite good. This is expected, since only a few SP energies are affected by the approximation, and thus they should contribute with a small deviation to the final energy.

Calculations of the same type with a different number of major oscillator shells differ considerably. The calculations with $e_{\text{Max}} = 12$ and $l_{\text{Max}} = 10$ are the most accurate as they employ the largest bases. An investigation of the energy gain by including more shells, shown in Fig. 8, suggests that convergence has not yet been reached and considerable changes may occur if even more shells are included.

To estimate the contributions originating from the inclusion of more shells, which is computationally not practicable, we perform an exponential fit of the form

$$E^{(0+2)}(e_{\text{Max}}) = a \exp(-b \cdot e_{\text{Max}}) + c , \qquad (4.3)$$

with the fit parameters a,b, and c. Some representative fits are displayed in Fig. 9. For $e_{\text{Max}} \to \infty$ we obtain the ground state energies displayed in Fig. 8. For nuclei up to ${}^{56}\text{Ni}$ the predicted values seem reasonable. For heavier nuclei the extrapolation seems to overestimate the binding energies. The exponential fit provides only a rough estimate of convergence behavior, and is probably an unappropriate choice for ${}^{78}\text{Ni}$, ${}^{88}\text{Sr}$ and ${}^{90}\text{Zr}$. Bases used to determine the fit parameters are less reliable for heavier nuclei, and the energy gain for larger orbital bases might no longer follow a sufficiently uniform

⁹Experimental values are always marked by bars in the graphs.



Figure 8: Binding energies from HFC ED MBPT calculations with $e_{\text{Max}} = 6, 8, 10$, and $e_{\text{Max}} = 12$ with $l_{\text{Max}} = 10$ (in this order: $(\bigcirc)(\blacksquare)(\bigstar)(\bigstar)$). Extrapolated values obtained from an exponential fit (\bigcirc) .



Figure 9: Convergence behavior of binding energies. The graph displays the some exemplatory fits (¹⁶O,⁴⁰Ca,⁵⁶Ni,⁹⁰Zr). The data points are calculated by HF+MBPT HFC method with $e_{\text{Max}} = 6, 8, 10$, and $e_{\text{Max}} = 12$ with additional restriction $l_{\text{Max}} = 10$.

scheme¹⁰. Moreover, it seems that second-order MBPT tends to over-estimate binding energies [17], and this effect is likely compensated by higher order MBPT contributions.

In conclusion, we find that the exact-denominator (ED) method yields in general better results. Still, the correction to the approximated-denominator (AD) method can be considered a "fine tuning" compared to the typical deviations between different approxmation methods, e.g. RPA.

5. Corrections for Single-Particle (SP) Energies

In this section corrections to the HF single-particle (SP) energies are calculated. Again we employ MBPT as a tool to estimate the impact of long-range correlations.

5.1. Estimating Single-Particle Energies

To calculate the SP energy of a given level we take the energy differences of two systems, one with N-particles and the other with (N - 1)-particles.

We first suppose a *N*-particle system in the many-body state $|^{N}\Psi_{0}\rangle$ with energy ^{N}E . Now we subtract the energy $^{N-1}E_{c}$ of a (N-1)-particle system in state $|^{N-1}\Psi_{c}\rangle$, where nucleon *c* is missing. The unperturbed Hamiltonian is chosen to be the HF Hamiltonian and energy corrections up to second order are considered ($^{N}E \approx {}^{N}E^{(0+1+2)}$, ${}^{N-1}E_{c} \approx {}^{N-1}E_{c}^{(0+1+2)}$):

$$\begin{aligned} \varepsilon_c' &= {}^{N} E^{(0+1+2)} - {}^{N-1} E_c^{(0+1+2)} = \\ &= ({}^{N} E^{(0)} + {}^{N} E^{(1)} + {}^{N} E^{(2)}) - ({}^{N-1} E_c^{(0)} + {}^{N-1} E_c^{(1)} + {}^{N-1} E_c^{(2)}) = \\ &= {}^{N} E^{\text{HF}} - {}^{N-1} E_c^{(0)} - {}^{N-1} E_c^{(1)} + {}^{N} E^{(2)} - {}^{N-1} E_c^{(2)} , \end{aligned}$$
(5.1)

where the HF energy ${}^{N}E^{\rm HF}$ includes the zeroth and the first order of MBPT energies. We have to stress that we do *not* do standard MBPT for the (N-1)-particle system, since an approximation is made in representing the zeroth-order wave function of the (N-1)-particle system by the N-particle HF ground state Slater determinant, removing the particle of SP level c. In general, the HF SP levels of the N-particle system are not equal, but merely similar, to the orbitals of the (N-1)-particle system. Yet this simplification leads to a tremendous reduction of the sums later on.

Applying this ansatz to our many-body Hamiltonian the energy contributions organized by perturbation order are given by

¹⁰The fitting points of the last three nuclei lie nearly on a straight line. Thus, a minimal deviation (esp. of the last one) affects considerably the over-all curvature of the exponential fit.

5. Corrections for Single-Particle (SP) Energies

$${}^{N}E^{(0)} - {}^{N-1}E^{(0)} + {}^{N}E^{(1)} - {}^{N-1}E^{(1)} = \varepsilon_{c}$$

$${}^{N}E^{(2)} = \sum_{\mathcal{N}} \frac{\left|\left\langle^{N}\Psi_{0}\right| \operatorname{H_{int}}\left|\mathcal{N}\right\rangle\right|^{2}}{\left\langle^{N}\Psi_{0}\right| \operatorname{H_{int}}\left|{}^{N}\Psi_{0}\right\rangle - \left\langle\mathcal{N}\right| \operatorname{H_{int}}\left|\mathcal{N}\right\rangle} =$$

$$= \frac{1}{4} \sum_{a,b,r,s} \frac{\left|\left\langle^{N}\Psi_{0}\right| \operatorname{H_{int}}\left|{}^{N}\Psi_{ab}\right\rangle\right|^{2}}{{}^{N}E^{(0)} - {}^{N}E^{(0)}rs}} = \frac{1}{4} \sum_{a,b,r,s} \frac{\left|\left\langle ab\right| \operatorname{H_{int}}\left|rs\right\rangle\right|^{2}}{\mathcal{Z}} (5.3)$$

$${}^{N-1}\!E^{(2)} = \sum_{\mathcal{N}} \frac{\left|\left\langle^{N-1}\Psi_{c}\right| \operatorname{H_{int}}\left|\mathcal{N}\right|^{2}}{\left\langle^{N-1}\Psi_{c}\right| \operatorname{H_{int}}\left|\mathcal{N}\right\rangle - \left\langle\mathcal{N}\right| \operatorname{H_{int}}\left|\mathcal{N}\right\rangle}$$

$$(5.4)$$

with

$$\mathcal{Z} = \sum_{d} \langle da | \operatorname{H}_{\operatorname{int}} | da \rangle + \sum_{d \neq a} \langle db | \operatorname{H}_{\operatorname{int}} | db \rangle -$$

$$- \sum_{d}^{a \to r, b \to s} \langle dr | \operatorname{H}_{\operatorname{int}} | dr \rangle - \sum_{d \neq r}^{a \to r, b \to s} \langle ds | \operatorname{H}_{\operatorname{int}} | ds \rangle .$$
(5.5)

 ε_c denotes the HF SP energy. \mathcal{N} runs over all possible excitations of the N-particle system or the (N-1)-particle system respectively. The latin letters denote occupied and unoccupied states as stated in Sec. 3.1. Eq. 5.3 is just the second order MBPT term as in Sec. 3. The first-order contributions in Eq. 5.2 are the same for the N-particle and the (N-1)-particle system as a consequence of Koopman's theorem [10]. Thus to find the lowest contributing order corrections, we subtract second-order energies of both particle systems.

In preparation for the subtraction, we split the second-order contributions of the (N-1)-particle system (Eq. 5.4) by excitation type:

A) Single excitations $|^{N-1}\Psi_{ca}^{r}\rangle$: These include all excitations $a \to r$. Despite of Brillouin's theorem these excitations do contribute to the energy correction, since they allow the levels of the (N-1)-particle system¹¹ to "relax", and therefore make them closer to the optimum SP levels. The resulting contribution reads:

$${}^{N-1}E_{\mathcal{A}}^{(2)} = \sum_{a,r}^{\star} \frac{\left|\left\langle {}^{N-1}\Psi_{c}\right| \operatorname{H}_{\operatorname{int}} \left| {}^{N-1}\Psi_{ca} \right. \right\rangle\right|^{2}}{\frac{1}{2} \sum_{d,e}^{\star} \left\langle de\right| \operatorname{H}_{\operatorname{int}} \left| de \right. \right\rangle - \frac{1}{2} \sum_{d,e}^{a \to r,\star} \left\langle de\right| \operatorname{H}_{\operatorname{int}} \left| de \right. \right\rangle}{\left| e^{2} \right|^{2}} = \sum_{a \neq c,r} \frac{\left|\left\langle ac\right| \operatorname{H}_{\operatorname{int}} \left| cr \right. \right\rangle\right|^{2}}{\sum_{d}^{\star} \left\langle da\right| \operatorname{H}_{\operatorname{int}} \left| da \right. \right\rangle - \sum_{d}^{a \to r,\star} \left\langle dr \right| \operatorname{H}_{\operatorname{int}} \left| dr \right. \right\rangle}$$
(5.6)

All of the above sum indices which cannot be equal c are marked with a star \star .

¹¹These levels are (in the applied approximation) the HF levels of the N-particle system.

5. Corrections for Single-Particle (SP) Energies

B) Double excitations of type $|^{N-1}\Psi_{cab}^{rs}\rangle$: Include all excitations $a \to r$ and $b \to s$. This is the usual type of excitations which occur in MBPT – only that $a, b \neq c$. Thus we find

$${}^{N-1}\!E_{\mathcal{B}}^{(2)} = \frac{1}{4} \sum_{a,b,r,s}^{\star} \frac{\left|\left\langle ab\right| \operatorname{H}_{\mathrm{int}} \left| rs \right\rangle\right|^{2}}{\frac{1}{2} \sum_{d,e}^{\star} \left\langle de\right| \operatorname{H}_{\mathrm{int}} \left| de \right\rangle - \frac{1}{2} \sum_{d,e}^{a \to r,b \to s,\star} \left\langle de\right| \operatorname{H}_{\mathrm{int}} \left| de \right\rangle} = \frac{1}{4} \sum_{a,b,r,s}^{\star} \frac{\left|\left\langle ab\right| \operatorname{H}_{\mathrm{int}} \left| rs \right\rangle\right|^{2}}{\mathcal{X}},$$

$$(5.7)$$

where $\mathcal{X} \equiv \mathcal{Z}$ with the constraint that the sums do not run over c.

C) Double excitations of type $|^{N-1}\Psi_{cab}^{cr}\rangle$: Includes all excitations with $a \to c$ and $b \to r$. This type of excitations has to be considered in the (N-1)-particle system since excitations into the now unoccupied *c*-level occur. The sum writes

$${}^{N-1}E_{\mathcal{C}}^{(2)} = \frac{1}{2} \sum_{a,b,r}^{\star} \frac{\left|\left\langle {}^{N-1}\Psi_{c}\right| \operatorname{H_{int}}\left| {}^{N-1}\Psi_{cab} \right. \right|^{2}}{\left\langle {}^{N-1}\Psi_{c}\right| \operatorname{H_{int}}\left| {}^{N-1}\Psi_{c}\right\rangle - \left\langle {}^{N-1}\Psi_{cab} \right. \right|^{2}} = \\ = \frac{1}{2} \sum_{a,b,r}^{\star} \frac{\left|\left\langle ab\right| \operatorname{H_{int}}\left|cr\right\rangle\right|^{2}}{\frac{1}{2} \sum_{a,e}^{\star} \left\langle de\right| \operatorname{H_{int}}\left|de\right\rangle - \frac{1}{2} \sum_{a,e}^{a \to c,b \to r,\star} \left\langle de\right| \operatorname{H_{int}}\left|de\right\rangle} =$$
(5.8)
$$= \frac{1}{2} \sum_{a,b,r}^{\star} \frac{\left|\left\langle ab\right| \operatorname{H_{int}}\left|cr\right\rangle\right|^{2}}{\mathcal{Y}},$$

with

$$\mathcal{Y} = \sum_{d}^{\star} \langle da | \operatorname{H}_{\operatorname{int}} | da \rangle + \sum_{d \neq a}^{\star} \langle db | \operatorname{H}_{\operatorname{int}} | db \rangle -$$

$$- \sum_{d}^{a \to c, b \to r, \star} \langle dc | \operatorname{H}_{\operatorname{int}} | dc \rangle - \sum_{d \neq r}^{a \to c, b \to r, \star} \langle dr | \operatorname{H}_{\operatorname{int}} | dr \rangle .$$
(5.9)

When we approximate the denominators of the above terms, analogous as in Eq. 3.18, by differences in HF SP energies, the sums are tremendously reduced by cancellation and yield the following result:

$$\varepsilon_{c}' = \varepsilon_{c} + \frac{1}{2} \sum_{a,b,r} \frac{\left|\left\langle ab \right| \operatorname{H}_{\operatorname{int}} \left| cr \right\rangle\right|^{2}}{\varepsilon_{c} + \varepsilon_{r} - \varepsilon_{a} - \varepsilon_{b}} + \frac{1}{2} \sum_{a,r,s} \frac{\left|\left\langle rs \right| \operatorname{H}_{\operatorname{int}} \left| ca \right\rangle\right|^{2}}{\varepsilon_{c} + \varepsilon_{a} - \varepsilon_{r} - \varepsilon_{s}}$$
(5.10)

Note that the summations over a and b include the c-level as it is introduced to the final sum by the contribution of the single excitation terms.

This result, deduced by the simplest form of MBPT, can also be obtained by the most elementary approximation of the Green's Function formalism [10].

5.2. Calculations and Results of SP Energy Corrections

Some of the closed-shell nuclei were calculated with the AD SP energy corrections given by Eq. 5.10. The calculations were implemented with the HFM method with the same settings as the calculations in the last section.

Unphysically large correction-terms to the HF SP energies resulted by the AD calculations, mixing the energetical order of SP levels. Monitoring the individual contributions to the sums, large contributions (> 4 MeV) of only a few terms of the second term of Eq. 5.10 were observed. The large contributions usually had a small denominator (< 0.02 MeV). This could hint at some near-degeneracies evoked by inadequate approximations.

Comparing the denominators of first term and second term of Eq. 5.10 it is easily seen that in the second term the total denominator energy is at least equal to the Fermi gap. This does not hold true for the first term since this denominator involves the difference of a 2p state with a 1p1h state. Near-degeneracies can occur.

A hybrid version, a mixture of ED and AD sums, of the energy corrections was investigated.¹² The troublesome second term of Eq. 5.10, which contained the large sum terms, was substituted by the ED terms. Nevertheless, the results of this implementation yielded no improvement to the AD version. Some of the SP energies still were extremely large. The double excitations of type $C(|^{N-1}\Psi_{cab}^{cr}\rangle)$ have big contributions to SP energies. Omitting these excitations in the calculations correction energies of a reasonable range of about -2 to -8 MeV were obtained for selected closed-shell nuclei.

It seems that energy corrections to the HF SP energies are not tractable by simple MBPT.

6. Outlook

The binding energies obtained by a transformed realistic potential by applying, first, Hartree-Fock (HF) and then many-body perturbation theory (MBPT) were improved in Sec. 4. Within the range of deviation of distinct approximation methods this correction is small and systematical errors due to the restriction to two-body interactions are expected to yield greater inaccuracies.

So far, binding energies are already in a good agreement with the experiment. In contrast, there is less consistency concerning the charge radii and density distributions with current approximations. Presently investigation in the influence of tree-body interaction in this framework is done [14]. Considering the effects of three-body forces one expects a better consistency of the results, especially for observable like the charge radii.

There is also investigation in advanced HF versions to improve the description of long-range correlations. The HF Bogoliubov scheme [16] employs a *quasi-particle* approximation, whereas the Brückner scheme [15] unifies HF and MBPT before iterating it in a similar way to the standard HF iterations.

¹²The hybrid method, and not an completely ED method, was chosen to reduce calculation time.

6. Outlook

Regarding the single-particle (SP) energies it seems that more sophisticated approximation methods are needed. A promising ansatz is to treat this problem with Green's Function (GF) theory going beyond the simplest reduction of the Dyson equation¹³.

¹³F. Dyson introduced an effective energy-dependent (*self-energy*) potential. Moreover, he showed that the exact Green's Function can be written in an integral equation – the so-called Dyson equation. This expression can be expanded as a perturbation series in matrix representation. Applying GF theory with the Dyson equation results, when considering only effects up to second order, in Eq. 5.10, which is in Sec. 5 deduced by MBPT.

A. Slater rules

A. Slater rules

In this section we present a set of rules which allows us to easily evaluate matrix elements

$$\langle \Psi_1 | \mathcal{O} | \Psi_2 \rangle$$
 (A.1)

with states consisting of A-particle Slater determinants¹⁴ $|\Psi\rangle$ and operators that are a sum of one- or two-particle operators

$$\mathcal{O}_1 = \sum_{i=1}^A \mathcal{T}_i \tag{A.2}$$

$$\mathcal{O}_2 = \sum_{i=1}^A \sum_{j>i}^A \mathcal{V}_{ij} \equiv \sum_{i(A.3)$$

Those operators depend on the position, momentum, spin, and isospin of the involved particles.

The rules for evaluating the matrix elements depend on whether \mathcal{O} contains one- or two-body operators and, furthermore, to which degree the two determinants $|\Psi_1\rangle$ and $|\Psi_2\rangle$ differ. For one-body operators two nontrivial cases exist, for two-body operators there are three. We distinguish the following cases:

1. $|\Psi_1\rangle$ and $|\Psi_2\rangle$ are identical:

$$|\Psi_1\rangle = |\Psi_2\rangle \equiv |\Psi\rangle,$$

2. $|\Psi_1\rangle$ and $|\Psi_2\rangle$ differ by exactly one spin orbital:

$$|\Psi_1\rangle \equiv |\Psi\rangle, |\Psi_2\rangle \equiv |\Psi_a^{a'}\rangle,$$

3. $|\Psi_1\rangle$ and $|\Psi_2\rangle$ differ by exactly two spin orbitals:

$$|\Psi_1\rangle \equiv |\Psi\rangle, |\Psi_2\rangle \equiv |\Psi_a^{a'b'}\rangle$$

When two determinants differ by more SP states than the order x of the x-body operator, the matrix element is automatically zero, since the operator cannot couple those states.

To apply the Slater rules, the determinants have to be put in maximum coincidence by appropriate permutations of the SP states¹⁵.

We will present an exemplary deviation of one of the rules followed by a complete summary of the rules (Tab. 3 and 4). An A-nucleon Slater determinant containing the SP states

$$\underbrace{\frac{|i\rangle, |j\rangle, \dots, |k\rangle}{A}}_{A}$$

¹⁴As before, all considered states are supposed to be antisymmetric.

¹⁵E.g., by permutating the SP states of $|\Psi_2\rangle$ until all equal SP states appearing in $|\Psi_1\rangle$ and $|\Psi_2\rangle$ have pairwise the same position.

A. Slater rules

is defined as

$$\left|\Psi\right\rangle = (A!)^{-1/2} \sum_{n=1}^{A!} (-1)^{\mathbf{p}_n} \mathcal{P}_n\left\{\left|i\right\rangle \otimes \left|j\right\rangle \otimes \ldots \otimes \left|k\right\rangle\right\} , \qquad (A.4)$$

where A! is the number of possible permutations of the nucleons. \mathcal{P}_n is the *permutation* operator that generates the *n*th perturbation of the many-body state. p_n is the number of transpositions required to obtain this permutation.

Taking two determinants in maximum coincidence, we have

$$\langle \Psi_i | \Psi_j \rangle = (A!)^{-1} \sum_{i}^{A!} \sum_{j}^{A!} (-1)^{\mathbf{p}_i} (-1)^{\mathbf{p}_j} \cdot \mathcal{P}_i \left\{ \cdots \langle a | \otimes \langle b | \cdots \right\} \mathcal{P}_j \left\{ \cdots | a' \rangle \otimes | b' \rangle \cdots \right\} .$$

$$(A.5)$$

The SP states are assumed to form an orthonormal set. Thus the expression above is only non-zero if the primed 'SP states are identical to the unprimed ones and two many-body states $|\Psi_i\rangle$ and $|\Psi_j\rangle$ are orthogonal if they do not contain the identical SP states. Since the SP states are normalized we find $\langle \Psi_i | \Psi_i \rangle = 1$.

Let us now derive explicitly case 1 for a one-particle operator \mathcal{O}_1 . The matrix elements of $\mathcal{T}_1, \mathcal{T}_2, \mathcal{T}_3, \ldots$ are the same when the particles are indistinguishable, so

$$\left\langle \Psi \right| \mathcal{O}_{1} \left| \Psi \right\rangle = \left\langle \Psi \right| \sum_{i=1}^{A} \mathcal{T}_{i} \left| \Psi \right\rangle = A \left\langle \Psi \right| \mathcal{T}_{1} \left| \Psi \right\rangle =$$

$$= \frac{A}{A!} \sum_{i}^{A!} \sum_{j}^{A!} (-1)^{p_{i}} (-1)^{p_{j}} \cdot$$

$$\cdot \mathcal{P}_{i} \left\{ \cdots \left\langle a \right| \otimes \left\langle b \right| \cdots \right\} \mathcal{T}_{1} \mathcal{P}_{j} \left\{ \cdots \left| a' \right\rangle \otimes \left| b' \right\rangle \cdots \right\} ,$$

$$(A.6)$$

where we choose the operator for the first particle \mathcal{T}_1 by convention. In case 1 the primed SP states are the same as the unprimed. For the combination of the particles $2, 3, \ldots, A$ we obtain zero unless the particles are in the same level in the *i*th permutation as in the *j*th permutation. Given that all particles occupy the same levels the first particle also has to be in the same level in both of the permutations. Thus, the permutations have to be the same (i = j) to give a contribution:

$$\left\langle \Psi \right| \mathcal{O}_1 \left| \Psi \right\rangle = ((A-1)!)^{-1} \sum_{i}^{A!} \mathcal{P}_i \left\{ \cdots \left\langle a \right| \otimes \left\langle b \right| \cdots \right\} \mathcal{T}_1 \mathcal{P}_i \left\{ \cdots \left| a \right\rangle \otimes \left| b \right\rangle \cdots \right\} .$$
(A.7)

The combination of the particles 2, 3, 4, ... always yields 1 since the SP states are normalized. In the sum over A! permutations, particle 1 occupies each SP state (A-1)! times because there are (A-1)! ways to arrange the other particles among the remaining (A-1) SP states. This leads us to

$$\langle \Psi | \mathcal{T}_1 | \Psi \rangle = \sum_a \langle a | \mathcal{T}_1 | a \rangle \equiv \sum_a \langle a | \mathcal{T} | a \rangle$$
 (A.8)

B. Brief Description of BW MBPT

	$\mathcal{O}_1 = \sum_{i=1}^A \mathcal{T}_i$
Case 1:	$\langle \Psi \mathcal{O}_1 \Psi \rangle = \sum_a \langle a \mathcal{T} a \rangle$
Case 2:	$\left\langle \left. \Psi \right \mathcal{O}_1 \left \Psi_a^r \right. \right\rangle = \left\langle \left. a \right \mathcal{T} \left r \right. \right\rangle$
Case 3:	$\left\langle \left. \Psi \right \mathcal{O}_1 \left \Psi^{rs}_{ab} \right. \right\rangle = 0$

Table 3: Matrix elements between determinants for one-particle operators.

	$\mathcal{O}_2 = \sum_{i < j}^A \mathcal{V}_{ij}$
Case 1:	$\left\langle \Psi \right \mathcal{O}_2 \left \Psi \right\rangle = \frac{1}{2} \sum_{a,b} \left\langle \left. ab \right \mathcal{V} \left ab \right\rangle \right\rangle$
Case 2:	$\left\langle \left. \Psi \right \mathcal{O}_{2} \left \Psi_{a}^{r} \right. ight angle = \sum_{b} \left\langle \left. ab \right \mathcal{V} \left rb \right. ight angle$
Case 3:	$\left\langle \left. \Psi \right \mathcal{O}_{2} \left \Psi_{ab}^{rs} \right. \right\rangle = \left\langle \left. ab \right \mathcal{V} \left rs \right. \right\rangle$

Table 4: Matrix elements between determinants for two-particle operators.

as case 1 of the Slater rules for an one-particle operator.

B. Brief Description of BW MBPT

We introduce projection operators to separate the many-body Hilbert space into two subspaces: the *model space* with projector P and the residual space with projector Q with P + Q = 1 and PQ = QP = 0. We split the Hamiltonian according to $H = H_0 + W$, with $PH_0P = QH_0Q = H_0$. Our aim is to find an effective Hamiltonian H_{eff} which is restricted to the model space, $PH_{eff}P = H_{eff} = PH_0P + PW_{eff}P$, such that $H_{eff}P | E_n \rangle = E_nP | E_n \rangle$ for at least a few eigenvalues. Thus the effective Hamiltonian acting in model space should have the same eigenenergies E_n as the original Hamiltonian H, and eigenstates that are projections of the exact eigenstates. The effective residual perturbation W_{eff} can be defined recursively and depends on the (yet unknown) eigenvalue E_n :

$$W_{\text{eff}}(E_n) = W + WQ(E_n - H_0)^{-1}QW_{\text{eff}}(E_n) , \qquad (B.1)$$

To employ the BW MBPT for our purposes, we choose H_0 to be the diagonal matrix elements of H in the HF basis, and W = H – H₀ are therefore the off-diagonal matrix elements. The HF state $|E_n^{(0)}\rangle$ constructs our model space P = $|E_n^{(0)}\rangle\langle E_n^{(0)}|$, thus $Q = \sum_n |n\rangle\langle n| - |E_n^{(0)}\rangle\langle E_n^{(0)}|$ and $\langle E_n^{(0)}| H_0 |E_n^{(0)}\rangle = E_n^{(0)}$. The corrected energy is given by

$$E_n = \langle E_n^{(0)} | \mathcal{H}_0 | E_n^{(0)} \rangle + \langle E_n^{(0)} | \mathcal{W}_{\text{eff}} | E_n^{(0)} \rangle = E_n^{(0)} + E_{\text{corr},n} .$$
(B.2)

C. Implementation-specific Remarks

 $E_{\text{corr},n}$ can be expanded as a series:

$$E_{n} = E_{n}^{(0)} + \sum_{m} \frac{\left| \left\langle E_{n}^{(0)} \middle| W \middle| m \right\rangle \right|^{2}}{E_{n} - E_{m}^{(0)}} + \sum_{m,k} \frac{\left\langle E_{n}^{(0)} \middle| W \middle| m \right\rangle \left\langle m \middle| W \middle| k \right\rangle \left\langle k \middle| W \middle| E_{n}^{(0)} \right\rangle}{(E_{n} - E_{m}^{(0)}) \cdot (E_{n} - E_{k}^{(0)})} + \dots$$
(B.3)

As E_n appears in both sides of the definition, not permitting an algebraic solution, this equation requires a self-consistent method like an iterative scheme to be solved.

C. Implementation-specific Remarks

This section contains information and remarks concerning the implementation of the new routines into the *nsuite* project.

C.1. Changes to nsuite

- A new option check was introduced when parsing the command line of the files calcenergypt_hfm.c and calcenergypt_hfc.c. The added variable CMode specifies the "Calculation Mode":
 - 0: for the approximated-denominator (AD) method,
 - 1: for the exact-denominator (ED) method.
- Both versions, HFM and HFC, calculate the denominator utilizing the D2VTCenergies¹⁶. Choosing a different value for the binary sel-scheme does not (!) alter the calculation energies utilized to calculate the denominator, e.g. D2VC¹⁷, D2V¹⁸.

C.2. List of Modified (M) and Newly Created (C) Files

PTE_Calc_HFC.h (M): updated function declaration

PTE_Calc_HFC.c (M): added the m-averaged ED method

PTE_Calc_HFM.h (M): updated function declaration

PTE_Calc_HFM.c (M): added the standard ED method

calcenergypt_hfm.c (M): introduced the calculation mode CMode

calcenergypt_hfc.c (M): introduced the calculation mode CMode

PAR_Base.h (M): introduced calculation mode variable in PAR structure

¹⁶Second order MBPT energies (D2) which are calculated with a transformed Hamiltonian including NN-interactions (V), kinetic energy (T) and Coulomb interactions (C).

 $^{^{17}\}mathrm{Hamiltonian}$ includes only V and C.

¹⁸Hamiltonian includes only V.

D. Additional Graphs

PAR_Base.c (M): introduced calculation mode to functions

HFC_Base.h (M): added HFC.eeee to HFC_Struct

HFC_Base.c (M): initialized HFC.eeee

HFM_Base.h (M): added HFM.eeee to HFM_Struct

HFM_Base.c (M): initialized HFM.eeee

COE_* (C): calculation routine for SP energy corrections

calcorbiten_hfm (C): calculation routine for SP energy corrections

makefile (M): entries for compiling calcorbiten_hfm

libHF\makefile (M): entries for COE_*

D. Additional Graphs

In this section we present two graphs depicting exemplatory results of the SP energy corrections.



Figure 10: SP energies of protons and neutrons for ¹⁶O (HF and HF+Correction) are depicted. Left-hand-side with all terms of Eq. 5.10 and right-hand-side with double excitations of type $\mathcal{C}(|^{N-1}\Psi_{cab}^{cr}\rangle)$ omitted. (right-hand-side).





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Acknowledgement

My thanks goes to the supervising Prof. Dr. Robert Roth for the flexible and animating way of managing my Bachelor-Thesis, for the relaxed discussions about the topic, and for the open and pensive gaze, furrowing his brow, upon my two knocks on the doorframe before entering for "some short questions" more.

I thank Heiko Hergert for the helpfull instructions on the topic and his very accurate and constructive way of correcting. He used up at least one red-ink pen on my printouts.

I'd like to thank my roommate Pascal Büscher for good – off-physical – distractions and the theoretical nuclear physics groups THQ, NHQ and TNP++ for the harmonious working atmosphere on the fourth floor – never ate so much cake.

Finally, I want to thank my parents for their support and trust in me, for the intrest in my studies and the never-ending curious questions. I wouldn't be writing these lines without them.