Ab initio methods:
An introduction through many-body perturbation theory

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1 A short intro to many-body perturbation theory

We focus in the following on the application of many-body perturbation theory (MBPT) to closed-shell systems. As such, we start from a spherical Slater determinant reference state:

$$|\Phi\rangle \equiv \sum_{i=1}^{A} c_i^\dagger |0\rangle, \tag{1}$$

where the single-particle creation operators $c_i^\dagger$ act on the physical vacuum $|0\rangle$. For systems that do not exhibit a closed-shell behaviour, one will typically start from a more sophisticated reference state. We then normal-order the Hamiltonian with respect to $|\Phi\rangle$:

$$H = H^0 + \sum_{pq} H^1_{pq} : c_p^\dagger c_q : + \frac{1}{4} \sum_{pqrs} H^2_{pqrs} : c_p^\dagger c_q^\dagger c_s c_r : + \frac{1}{36} \sum_{pqrstu} H^3_{pqrstu} : c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s : + \dots . \tag{2}$$

Let us admit that $|\Phi\rangle$ is the solution of the Hartree-Fock equation. We partition the Hamiltonian into an unperturbed part H_0 and a residual part H_1 as follows:

$$H_0 = H - H_1 = E_0 + \sum_p e_p : c_p^\dagger c_p : \quad H_1 = \sum_{pqrs} H^2_{pqrs} : c_p^\dagger c_q^\dagger c_s c_r :, \tag{3}$$

where $\{e_p\}$ denote the single-particle energies obtained from the Hartree-Fock solution.[1] One can write the correction to the ground-state energy as follows:

$$\Delta E = \langle \Phi | H_1 \sum_{n=1}^{\infty} (R H_1)^n | \Phi \rangle, \tag{4}$$

with the resolvent operator:

$$R \equiv \sum_a{}' \frac{|\Phi_a\rangle\langle\Phi_a|}{E^{(0)} - E_a^{(0)}}, \tag{5}$$

where the sum runs over particle states only. In the following and for convenience, we switch for the more convenient notation for the antisymmetrized two-body matrix element of the Hamiltonian operator $\bar{v}_{pqrs}$ where we immediately drop the bar and end up with v_{pqrs}.

[1] Overall, this corresponds to a Rayleigh-Schrödinger many-body perturbation theory with Møller-Plesset partitioning. See e.g. [1, 2] for a recent application of Brillouin-Wigner perturbation theory.

2 Second-order perturbation theory

The second-order contribution to the ground-state energy of the system reads as[2]

$$E^{(2)} = -\frac{1}{4}\sum_{abij}\frac{v_{abij}v_{ijab}}{\epsilon_{ab}^{ij}}, \tag{6}$$

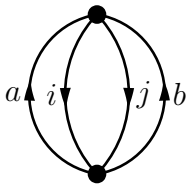
where we have introduced the standard notation

$$\epsilon_{ab\ldots}^{ij\ldots} = e_a + e_b + \cdots - e_i - e_j - \ldots, \tag{7}$$

where $a, b, \ldots$ denote the particle states (unoccupied in the reference state) and $i, j, \ldots$ denote hole states (occupied in the reference state).

Question 1. *Look at the denominator in the expression above. What happens if e_a, e_b have similar values as e_i, e_j? What does this mean in terms of physics?*

The second-order ground-state energy contribution is usually associated to the following diagram:[3]



The diagram respects the following rules:

- Each vertex is associated to a matrix element of the Hamiltonian, so a n-th order diagram has n vertices.
- The diagram is connected, i.e. each vertex is connected to all others by a series of hole/particle lines.
- Each propagator carries a certain quasi-particle label:
  - A hole line if going down.
  - A particle line if going up.
- As the Hamiltonian conserves the number of particle, each vertex is connected to two lines going in, and two lines going out (i.e. two annihilation and two creation operators).

The diagrammatic rules are built in such a way that obtaining all contributions at a given order correspond to generating all diagrams that respect the rules. Here at order two this is quite trivial, but we will see that it gets more complicated with every additional order.

It can be useful if one wants to discuss in details the diagrammatic contributions to introduce some concepts from graph theory:

Definition A graph $G = (V, E, \psi)$ is *connected* if for any pair of nodes there is a path connecting them.

[2]The absence of contribution from the one-body part of the Hamiltonian here is directly linked to our choice of reference state and partitioning.

[3]This type of diagram is called Hugenholtz diagram. Another pretty common type of diagrams is Goldstone diagrams, where vertices are expanded into two half vertices with an internal dashed line.

Definition Let $G = (V, E, \psi)$ be a graph. The *adjacency matrix* $A(g)$ is the $|V| \times |V|$ matrix with entries

$$a_{ij} = \left|\{e_k \in E \,:\, e_k \,\text{connects}\, v_i, v_j\}\right|.$$

In the case of our second-order MBPT diagram, this means:

$$A = \begin{pmatrix} 0 & 4 \\ 4 & 0 \end{pmatrix} \tag{8}$$

For oriented graphs (i.e. edges have a given start- and end-vertex) the definition needs to be slightly extended:

Definition Let $G = (V, E, \psi)$ be an oriented graph. The *oriented adjacency matrix* $\tilde{A}(g)$ is the $|V| \times |V|$ matrix with entries

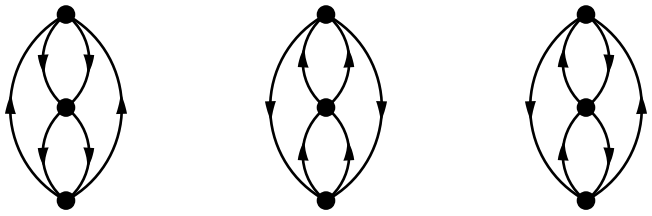
$$\tilde{a}_{ij} = \left|\{e_k \in E \,:\, e_k \,\text{goes from}\, v_i \,\text{to}\, v_j\}\right|.$$

For our MBPT diagram, this means:

$$\tilde{A} = \begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix} \tag{9}$$

3 Third-order perturbation theory

The three diagrams appearing at third order in MBPT are often called hole ladder, particle ladder, and ring diagram, and are displayed below:



Question 2. *Can you transcribe those order 3 diagrams into unoriented adjacency matrices?*

Question 3. *Can you transcribe those order 3 diagrams into oriented adjacency matrices?*

Question 4. *Can you figure out some rules that the matrices have to respect to be valid? Can you connect those rules to properties of the theory? What happens if you look at them in terms of rows and columns?*

Question 5. *The expressions for the three diagrams are given below (up to a sign). Can you figure out to which elements in the diagram the prefactors correspond?*

The differences in prefactors correspond to different combinations of contractions when you derive the expressions by hand with Wick's theorem, that eventually correspond to identical terms once you do the proper permutations and relabelling using the antisymmetry properties of your vertices. Diagrams elegantly resum them, leading directly to a more compact representation.

$$E^{(3)}_{\text{ring}} = \frac{1}{(2!)^3} \sum \frac{v_{abij} v_{ijkl} v_{klab}}{\epsilon^{ij}_{ab}\ \epsilon^{kl}_{ab}} \tag{10}$$

$$E^{(3)}_{\text{ring}} = \frac{1}{(2!)^3} \sum \frac{v_{abij} v_{cdab} v_{ijcd}}{\epsilon^{ij}_{ab}\ \epsilon^{ij}_{cd}} \tag{11}$$

$$E^{(3)}_{\text{ring}} = \sum \frac{v_{abij} v_{icak} v_{jkbc}}{\epsilon^{ij}_{ab}\ \epsilon^{jk}_{bc}} \tag{12}$$

$$\tag{13}$$

4 Fourth-order perturbation theory

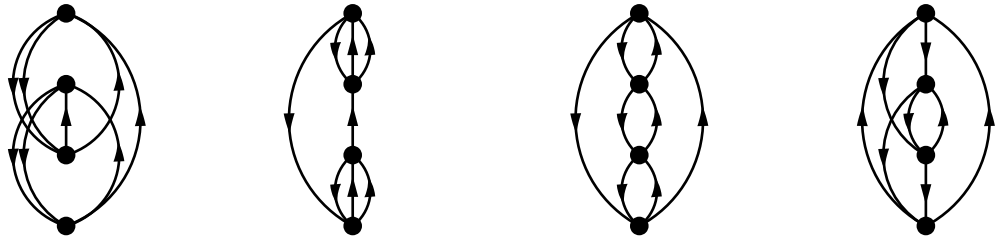
Question 6. *From the four-by-four adjacency matrices below, can you spot which ones are not good candidates for MBPT diagrams?*

$$\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 2 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 3 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \\ 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \end{pmatrix} \tag{14}$$

You should be able to connect the values of the matrix elements to properties of the diagrams. If it helps, do not hesitate to draw the diagram associated to each matrix. Do you notice anything off? Are there additional rules that you might have missed earlier?

Question 7. *Can you write (some of) the unoriented adjacency matrices corresponding to order four diagrams? The oriented ones? (Hint: There are 39 valid diagrams at order 4)*

Question 8. *Take a look at the four (valid) fourth-order diagrams below. If you had to categorise them as "single", "double", "triple" and "quadruple", what would be your guess?*



This notion of single, double, etc., excitation corresponds to the fact that the diagram connects states that are linked to the reference state via a 1p-1h, 2p-2h, etc., excitation. It connects the MBPT diagrammatic to the configuration-interaction expansion of the wave-function:

$$|\Psi\rangle = c_0|\Phi\rangle + \sum_{ai} c_a^i|\Phi_a^i\rangle + \sum_{abij} c_{ab}^{ij}|\Phi_{ab}^{ij}\rangle + \sum_{abcijk} c_{abc}^{ijk}|\Phi_{abc}^{ijk}\rangle + \dots \tag{15}$$

Also, note that these correspond to the singles, doubles, triples, etc., that appear in the names of couple cluster theory truncation schemes (CCD, CCSD, CCSDT...), as those different orders correspond to resuming all diagrams from a given category to infinite orders in MBPT. This explains why CC and other non-perturbative methods are powerful: they resum infinite series of MBPT diagrams and as such incorporate non-trivial physics contributions.

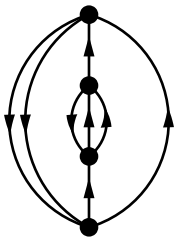
Question 9. *Take a look back at the second- and third-order diagrams. Under which category would they fall?*

Given the fast-growing number of diagrams, finding them all by hand becomes very soon particularly difficult. As such, generating them automatically is an appealing strategy. One way to do that is to generate all matrices that code for the MBPT diagrams.

Question 10. *Propose a schematic algorithm to generate all fourth-order adjacency matrices. Do you see easy ways to avoid paying the full cost of a brute force generation?*

Question 11. *Can you figure out the expression of the diagram showed below? Could you write out a set of rules to extract the expression of a diagram from its representation? Have a look at the expressions in order two and three to guide you.*[4] *(Hint: For the product of energy differences in the denominator, you will need to draw some horizontal lines through the diagrams)*

[4]Here we do not discuss the sign of a specific contribution, which requires setting a convention for the specific ordering of particle/hole labels at a vertex and the counting of the number of loops on the particle and hole lines. Though this is conveniently done by expanding the diagrams into antisymmetrised Goldstone diagrams (ASG), it can technically be done from the Hugenholtz diagrams, contrary to what is often stated.



5 A bit more advanced...

Question 12. *Can you figure out the numerical scaling of a code that would implement fourth-order MBPT in terms of N_h the number of hole states and N_p the number of particle states in your model space?*

Question 13. *If you were to extend things to three-body forces, can you think of things that would need to be changed?*

6 Additional bibliography

To learn more about ab initio methods as a whole and MBPT in particular, I recommend the following textbooks and publications:

- Shavitt and Bartlett have written the reference textbook on MBPT and Coupled-Cluster methods, though it focuses on the needs of quantum chemists [3].
- Tichai and collaborators have a nice and short review on perturbation theories for finite nuclei [4].
- The reviews by Hergert [5] and Soma [6] are good overall introductions to *ab initio* methods.
- Automated diagrammatic methods have been used for a while in chemistry and condensed matter [7–15] but have known a recent resurgence in nuclear physics [2, 16–20].
- The Oak Ridge - Tennessee group has recently published a simple many-body example code on a momentum lattice, covering Hartree-Fock, Coupled Cluster Theory and the In-Medium Similarity Renormalization Group [21].

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