Week 45: Many-body perturbation theory

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Topics to be covered

1. Thursday:
   1. Time-independent perturbation theory: examples of contributions in perturbation theory and diagrammatic representations
   2. Diagram rules and their derivations

2. Friday:
   1. Diagram examples
   2. Linked diagram theorem

3. Exercises week 45 at
   https://github.com/ManyBodyPhysics/FYS4480/blob/master/doc/Exercises/2025/Exercisesweek45.pdf

4. Lecture Material: Whiteboard notes (see above) and Shavitt and Bartlett chapters 5-7

Second midterm

The second midterm will be available from Friday November 14 with deadline November 24. We hope this will not interfere too much with other activities.

Reminder: Normal Ordering (Wick Setup)

Normal ordering $: \cdots :$ means: move all creation operators to the left of all annihilation operators *with a sign* for each fermionic swap.
For example,

$$: \hat{a}_p^\dagger \hat{a}_q : = \hat{a}_p^\dagger \hat{a}_q, \qquad : \hat{a}_q \hat{a}_p^\dagger : = -\hat{a}_p^\dagger \hat{a}_q. \tag{1}$$

Important subtlety: normal ordering must be defined with respect to a reference state. In many-body theory we *do not* always normal order relative to the true vacuum $|0\rangle$, but often relative to a filled Fermi sea $|\Phi_0\rangle$. We denote normal ordering with respect to $|\Phi_0\rangle$ by $N[\cdots]$ when we need to stress it.

Contractions (Fermions)

Given two fermionic operators $\hat{A}$ and $\hat{B}$, their **contraction** with respect to $|\Phi_0\rangle$ is defined as

$$\overbracket{\hat{A}\hat{B}} \equiv \langle\Phi_0| T(\hat{A}\hat{B}) |\Phi_0\rangle - \langle\Phi_0| N[\hat{A}\hat{B}] |\Phi_0\rangle, \tag{2}$$

where T is an ordering operation appropriate to the context.

For **time-independent** perturbation theory, we typically consider static (equal-time) operators in products like $\hat{V}\hat{V}\cdots\hat{V}$. Then the contraction between $\hat{a}_p$ and $\hat{a}_q^\dagger$ is

$$\overbracket{\hat{a}_p \hat{a}_q^\dagger} = \langle\Phi_0|\hat{a}_p\hat{a}_q^\dagger|\Phi_0\rangle = \delta_{pq} \times \begin{cases} 1, & p \text{ unoccupied in } |\Phi_0\rangle, \\ 0, & p \text{ occupied in } |\Phi_0\rangle. \end{cases} \tag{3}$$

Similarly,

$$\overbracket{\hat{a}_p^\dagger \hat{a}_q} = \langle\Phi_0|\hat{a}_p^\dagger\hat{a}_q|\Phi_0\rangle = \delta_{pq} \times \begin{cases} 1, & p \text{ occupied in } |\Phi_0\rangle, \\ 0, & p \text{ unoccupied in } |\Phi_0\rangle. \end{cases} \tag{4}$$

In words: a contraction "projects" whether an index is occupied (hole line) or unoccupied (particle line) in $|\Phi_0\rangle$.

Wick's Theorem (Static Form)

Wick's theorem for fermions states:
Any product of fermionic creation and annihilation operators can be written as a sum of

- a normal-ordered product $N[\cdots]$ (with respect to $|\Phi_0\rangle$),
- plus all possible normal-ordered products with one contraction,
- plus all with two contractions,
- etc.,
- up to the fully contracted term(s).

Symbolically,

$$
\hat{A}_1 \hat{A}_2 \cdots \hat{A}_n = N[\hat{A}_1 \hat{A}_2 \cdots \hat{A}_n] + \sum_{\substack{1 \text{ contraction}}} N[\cdots] + \sum_{\substack{2 \text{ contractions}}} N[\cdots] + \cdots
\tag{5}
$$

with appropriate fermionic signs for each reordering needed to realize the contractions.

Expectation Values and Full Contractions

Take the expectation value in $|\Phi_0\rangle$. Because all normal-ordered terms annihilate $|\Phi_0\rangle$ on the right (or $\langle\Phi_0|$ on the left), only *fully contracted* terms survive:

$$\langle\Phi_0|\hat{A}_1\hat{A}_2\cdots\hat{A}_n|\Phi_0\rangle = \sum_{\text{all complete pairings}} (\pm) \prod_{\text{pairs } (i,j)} \overbrace{\hat{A}_i\hat{A}_j}. \qquad (6)$$

Key point:

- The sum runs over all distinct ways of pairing operators into contractions.
- Each pairing comes with a fermionic sign determined by how many swaps are needed to bring operators next to each other.

This is the algebraic origin of Feynman- or Goldstone-like diagrams: each full contraction pattern $\leftrightarrow$ one diagram.

Many-Body Perturbation Theory (Energy)

For a non-degenerate reference state $|\Phi_0\rangle$ with unperturbed energy $E_0^{(0)}$, the Rayleigh–Schrödinger perturbation series for the ground-state energy is

$$E_0 = E_0^{(0)} + E_0^{(1)} + E_0^{(2)} + \cdots \tag{7}$$

with

$$E_0^{(1)} = \langle \Phi_0 | \hat{V} | \Phi_0 \rangle, \tag{8}$$

$$E_0^{(2)} = \sum_{n \neq 0} \frac{\left| \langle \Phi_n | \hat{V} | \Phi_0 \rangle \right|^2}{E_0^{(0)} - E_n^{(0)}}, \quad \text{etc.} \tag{9}$$

In second quantization, these matrix elements are operator strings of $\hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a}$ etc.

Wick's theorem

Wick's theorem reduces them to sums of complete contractions, with denominators from intermediate states. Each such contraction pattern corresponds to one diagram in the standard diagrammatic expansion of the ground-state energy.

Short summary

- Fermionic operators anticommute, and states are built as Slater determinants.
- The Hamiltonian is expressed in normal-ordered two-body form.
- Contractions encode occupied/unoccupied structure of the reference state.
- Wick's theorem rewrites any operator product as a sum over normal-ordered pieces plus contractions.
- Only fully contracted pieces survive in expectation values, and each full contraction $\leftrightarrow$ a diagram.

Next we will prove the **diagram rules**: how to translate any fully contracted term into a sign, symmetry factor, energy denominator, and algebraic expression.

From Contractions to Lines

Consider a two-body interaction vertex from $\hat{V}$:

$$\hat{V} = \frac{1}{4} \sum_{pqrs} \bar{v}_{pqrs} \, \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r. \tag{10}$$

A single insertion of $\hat{V}$ acting on $|\Phi_0\rangle$ can *excite* two particles from occupied (hole) states i, j to unoccupied (particle) states a, b. Schematically:

$$\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i \, |\Phi_0\rangle \quad \Rightarrow \quad |\Phi_{ij}^{ab}\rangle \, .$$

In diagrams:

- Each $\hat{a}^\dagger$ corresponds to an outgoing particle line.
- Each $\hat{a}$ corresponds to an incoming hole line.

A contraction between $\hat{a}_i$ in one vertex and $\hat{a}_a^\dagger$ in another vertex becomes a **line** connecting two vertices.

Sign Structure: Fermionic Minus Signs

When we evaluate a string like

$$\hat{a}_{p_1}^\dagger \hat{a}_{p_2}^\dagger \hat{a}_{q_2} \hat{a}_{q_1} \hat{a}_{r_1}^\dagger \hat{a}_{r_2}^\dagger \hat{a}_{s_2} \hat{a}_{s_1} \cdots$$

we must bring operators next to each other to form contractions. Every swap of two fermionic operators contributes a factor (-1).
Result: Each complete contraction pattern produces

$$(\text{sign}) = (-1)^{N_{\text{perm}}}, \tag{11}$$

where N_{perm} is the number of permutations needed to realize that pairing.
Diagrammatically: following standard fermionic diagram conventions, internal lines that "cross" encode these permutations. Thus, the sign of a diagram is the sign of the underlying antisymmetry of the many-body wave function.

Energy Denominators (Time-Independent PT)

In ordinary Rayleigh–Schrödinger perturbation theory, an nth-order energy correction involves n insertions of $\hat{V}$ and $(n-1)$ sums over intermediate states:

$$E_0^{(n)} = \sum_{\text{int. states}} \frac{\langle \Phi_0 | \hat{V} | \Phi_1 \rangle \langle \Phi_1 | \hat{V} | \Phi_2 \rangle \cdots \langle \Phi_{n-1} | \hat{V} | \Phi_0 \rangle}{(E_0^{(0)} - E_1^{(0)})(E_0^{(0)} - E_2^{(0)}) \cdots (E_0^{(0)} - E_{n-1}^{(0)})}. \tag{12}$$

Each intermediate state $|\Phi_k\rangle$ is a Slater determinant with some set of particle-hole excitations. Its unperturbed energy $E_k^{(0)}$ is just the sum of single-particle energies of occupied orbitals in that determinant.
Diagram rule: Every diagram at order n carries a product of denominators, one for each "time slice" (or intermediate configuration) in which a set of particle-hole excitations propagates.

Putting It Together: Generic Fermion Diagram Rule

For ground-state energy corrections in time-independent MBPT:

Rule 1: Vertices. Each interaction vertex contributes a factor $\bar{v}_{pqrs}$ with two incoming (hole) lines and two outgoing (particle) lines, summed over all internal indices.

Rule 2: Lines. Each internal line corresponds to a contraction and implies

- a Kronecker delta enforcing index matching,
- whether that index is a particle (unoccupied in $|\Phi_0\rangle$) or a hole (occupied in $|\Phi_0\rangle$),
- an energy associated with that orbital.

Putting It Together: Generic Fermion Diagram Rule

Rule 3: Signs. Include a global factor $(-1)^{N_{\text{perm}}}$ coming from the reordering of fermion operators needed to realize the contraction pattern. Equivalently: track the number of fermionic line exchanges.

Rule 4: Denominators. For an nth-order diagram, write down the sequence of intermediate Slater determinants generated as you "move through" the vertices. For each nontrivial intermediate determinant, include a denominator $[E_0^{(0)} - E_{\text{int}}^{(0)}]^{-1}$.

Example: Second-Order Correlation Energy

Consider the standard second-order (MP2-like) correlation energy.
Occupied indices: i, j. Unoccupied (virtual) indices: a, b.
The algebra from Eq. (12) gives

$$E_0^{(2)} = \frac{1}{4} \sum_{ijab} \frac{|\bar{v}_{ijab}|^2}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}, \tag{13}$$

where ϵ_p are single-particle energies from $\hat{H}_0$.

Diagrammatically:

- One vertex excites $ij \to ab$,
- The other vertex de-excites $ab \to ij$,
- Internal lines connect $i \leftrightarrow i$, $j \leftrightarrow j$, $a \leftrightarrow a$, $b \leftrightarrow b$,
- The denominator is the energy difference of the intermediate $2p$–$2h$ excitation,
- The sign is $+$ for this canonical ordering.

This diagram encodes the full sum over ($ijab$).

Symmetry / Combinatorial Factors

In higher orders, multiple distinct contraction patterns may generate the *same* topological diagram.

Rule 5 (Symmetry factor). If m different full contraction patterns reduce to the same topological diagram, that diagram receives a prefactor m (possibly with signs already accounted for).

Example:

- Two vertices with identical structure can sometimes be interchanged without changing the topology.
- Then both orderings appear separately in Wick expansions, so the diagram gains an extra factor 2.

This is how purely algebraic counting in Wick's theorem becomes combinatorics of diagrams.

Final Recipe (Ground-State Energy Diagrams)

To evaluate an *n*th-order fermionic diagram contributing to the ground-state energy:

1. Assign indices ($i, j, \ldots$ for occupied/hole, $a, b, \ldots$ for unoccupied/particle) to each line.

2. For each vertex, write a matrix element $\bar{v}_{pqrs}$ with appropriate indices from attached lines.

3. Multiply by the sign $(-1)^{N_{\text{perm}}}$ determined by fermion line permutations. This is the same as counting the number of hole lines and closed loops.

4. Sum over all internal indices (Einstein-like summation).

5. Include one energy denominator for every intermediate particle-hole configuration.

6. Multiply by the symmetry/combinatorial factor for that topological diagram.

Claim: These rules are *exactly* what you get by applying Wick's theorem to $\hat{V}^n$ between Slater determinants, collecting only fully contracted terms, and organizing them by topology.

Conceptual Proof Structure (Why This Works)

- Wick's theorem ensures: only full contractions survive in $\langle \Phi_0 | \hat{V}^n | \Phi_0 \rangle$.
- Each full contraction uniquely pairs annihilators with creators across the *n* interaction insertions.
- Each such pairing defines:
  - which particle-hole excitations appear,
  - in which order they propagate,
  - and how they recombine to $| \Phi_0 \rangle$.
- The fermionic anticommutation algebra enforces the correct sign.
- The intermediate-state sums naturally generate the denominators in Rayleigh–Schrödinger perturbation theory.
- Grouping algebraically equivalent contraction patterns gives topological diagrams plus symmetry factors.

Therefore, the diagram rules are not assumptions — they are a compact repackaging of Wick's theorem and standard many-body perturbation theory. More details follow here.

Lemma 1: Sign from Reordering

Statement. Let P be a pairing of indices $\{1, \ldots, 2n\}$ into n pairs (i,j) with $i < j$. Then

$$\langle \Phi_0 | T[\mathcal{O}] | \Phi_0 \rangle = \sum_P (-1)^{N_{\text{swaps}}(P)} \prod_{(i,j) \in P} \overbrace{O_i O_j},$$

where N_{swaps} is the number of adjacent anticommutations required to bring paired operators adjacent.

Proof sketch.

- Each exchange of two fermion operators introduces a factor -1.
- Bringing the operators into pair-adjacent form requires a finite number of adjacent swaps.
- The total sign is $(-1)^{N_{\text{swaps}}}$.

Lemma 2: Crossings and Sign Parity

Represent operator order on a horizontal line and draw arcs between paired operators:

$$(i, j) \rightarrow \text{arc connecting positions } i \text{ and } j.$$

Lemma: The parity of N_{swaps} equals the parity of the number of pairwise arc intersections:

$$(-1)^{N_{\text{swaps}}} = (-1)^{N_{\text{crossings}}}.$$

Proof sketch.

- Consider two pairs (i, j) and (k, ℓ) with $i < j$ and $k < \ell$.
- If $i < k < j < \ell$, the arcs cross.
- Each crossing corresponds to one swap of fermionic operators.

Corollary: Diagrammatically,

$$\text{sgn}(P) = (-1)^{N_{\text{crossings}}}.$$

Lemma 3: Closed Fermion Loops

Statement: Each closed fermion loop contributes an additional factor (-1).

Operator-level proof.

- A closed loop corresponds to a cyclic contraction such as $a_{p_1}^\dagger a_{q_1} a_{p_2}^\dagger a_{q_2} \cdots a_{p_m}^\dagger a_{q_m}$, where a_{q_m} contracts with $a_{p_1}^\dagger$.
- To perform this contraction, one operator must be moved past all other fermionic operators — an odd number of swaps.
- Hence, one factor of (-1) per closed fermion loop.

From Algebra to Diagrams

Phase rule for fermions:

$$\text{sgn}(P) = (-1)^{N_{\text{crossings}} + N_{\text{loops}}}.$$

Interpretation:

- Each line crossing $\Rightarrow$ one minus sign.
- Each closed fermion loop $\Rightarrow$ one minus sign.

Example:

- 2p–2h ladder: $N_{\text{crossings}} = 0$, $N_{\text{loops}} = 0 \Rightarrow$ sign $+1$.
- Particle-hole ring: $N_{\text{crossings}} = 0$, $N_{\text{loops}} = 1 \Rightarrow$ sign -1.

Counting Equivalent Contractions

Each perturbative order has:

$$E^{(n)} \sim \frac{1}{n!} \langle \Phi_0 | V \frac{Q}{E_0 - H_0} \cdots V | \Phi_0 \rangle.$$

The factor $1/n!$ comes from expansion of e^{-tV} or Dyson series.
When several Wick contractions yield the same topology:

$$S = |\mathrm{Aut}(\text{diagram})| \Rightarrow \text{include factor } \frac{1}{S}.$$

Final rule:

$$\text{Diagram weight} = \frac{(-1)^{N_{\text{crossings}} + N_{\text{loops}}}}{S} \text{ (product of matrix elements and denom}$$