# Week 45: Many-body perturbation theory

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# Week 45, November 3-7, 2025

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,

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

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:

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

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

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

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

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

where $N_{\mathrm{perm}}$ 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 $n$th-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 $(-1)^{N_{\mathrm{perm}}}$ 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 $n$th-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 $[E_0^{(0)} - E_{\mathrm{int}}^{(0)}]^{-1}$.

# 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

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

where $\epsilon_p$ 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 ($i, j, \dots$ for occupied/hole, $a, b, \dots$ 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 $(-1)^{N_{\mathrm{perm}}}$ 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 $N_{\text{swaps}}$ 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:

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

**Lemma:** The parity of $N_{\text{swaps}}$ 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 $(k,\ell)$ with $i<j$ and $k<\ell$.
- If $i<k<j<\ell$, the arcs cross.
- Each crossing corresponds to one swap of fermionic operators. A hole line represents such a swap.

**Corollary:** Diagrammatically,

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

# 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 $a^\dagger_{p_1} a_{q_1} a^\dagger_{p_2} a_{q_2} \cdots a^\dagger_{p_m} a_{q_m}$, where $a_{q_m}$ contracts with $a^\dagger_{p_1}$.
- 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:**

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

**Interpretation:**

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

**Example:**

- 2p–2h ladder: $N_{\mathrm{holes}} = 2$, $N_{\mathrm{loops}} = 2 \Rightarrow$ sign $+1$.
- 2nd-order Particle-hole ring: $N_{\mathrm{holes}} = 3$, $N_{\mathrm{loops}} = 1 \Rightarrow$ sign 1.

# Statement: Linked Diagram (Linked-Cluster) Theorem

**Theorem.** *For time-independent MBPT with intermediate normalization, the ground-state energy correction $\Delta E$ is given by the sum of linked (connected) vacuum diagrams only. Unlinked (disconnected) vacuum diagrams cancel order by order due to normalization and exponentiation.*

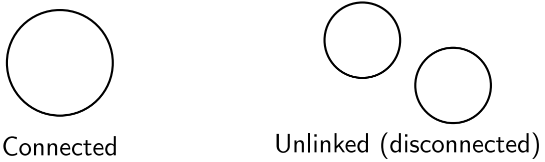
$$\boxed{\Delta E = \sum_{\text{connected vacuum diagrams}} (\text{value of diagram})}$$

Equivalently: if  is the sum of all (linked and unlinked) vacuum diagrams,

$$\log = \sum_{\text{connected vacuum diagrams}} ,$$

and the energy shift follows from the $\lambda$-derivative of log at $\lambda = 1$ (or from standard RS expressions).

# Connected vs. Unlinked: A Visual representation



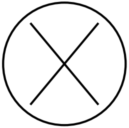

In algebra: products of lower-order *connected* contributions generate *unlinked* composites; these are precisely removed by the logarithm/normalization.

# Goldstone Diagrams for Energy: Examples

**Second order**

$$E^{(2)} = \sum_{\substack{ab\\ij}} \frac{|\langle ij||ab\rangle|^2}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

(one connected bubble)

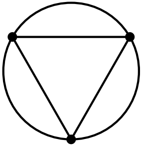


2nd order

**Third order**

$$E^{(3)} = \sum \frac{\langle\Phi||\nu\rangle\ \langle\nu||\mu\rangle\ \langle\mu||\Phi\rangle}{(E_0 - E_\nu^{(0)})(E_0 - E_\mu^{(0)})}$$

(topologies: ring, ladder, crossed-ladder)



3rd order (ring)

# Practical Notes for Calculations

- Prefer normal-ordered Hamiltonians; $E^{(1)}$ often vanishes for HF reference.
- Automate diagram generation: enumerate topologies, compute symmetry factors, energy denominators, and index sums.
- Check size-extensivity: only linked diagrams ensure correct scaling with particle number.
- Cross-validate: numerical MBPT vs. coupled-cluster (which sums linked *connected* diagrams to infinite order via exponentiation of the cluster operator).

# Take-Home Messages

- The linked (connected) nature of contributing diagrams to $\Delta E$ follows from general combinatorics (cumulants).
- Unlinked diagrams exponentiate and cancel via normalization $\Rightarrow$ size-extensive energies.
- The theorem guides practical many-body methods (MBPT, CC, MBPT-derived effective interactions).

For the proof, see either Shavitt and Bartlett chapter 6 and 7 or whiteboard notes.