Diagram Rules in Goldstone Diagrams and Linked Diagram Theorem

Time-Independent Fermionic Many-Body Perturbation Theory

FYS4480/9480

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Outline

Operator Algebra and Reference State

We work in the second-quantized representation:

$$\{a_p, a_q^\dagger\} = \delta_{pq}, \qquad \{a_p, a_q\} = 0, \qquad \{a_p^\dagger, a_q^\dagger\} = 0.$$

The reference determinant $|\Phi_0\rangle$ defines contractions:

$$a_p a_q^\dagger a_p a_q^\dagger \equiv \langle \Phi_0 | a_p a_q^\dagger | \Phi_0 \rangle = \delta_{pq}\, n_p,$$

where $n_p = 1$ for hole states, 0 for particle states.
A typical term in the MBPT expansion involves

$$\mathcal{O} = O_1 O_2 \cdots O_{2n}, \quad O_k \in \{a_p, a_q^\dagger\},$$

where each $(\mathrm{O}_k) is either (a_r) or (a_s^\dagger). Wick's theorem writes [\langle \Phi_0 | T[\mathcal{O}] | \Phi_0 \rangle = \sum_{\text{all pairings } P} \mathrm{sgn}(P) \prod_{\text{pairs } (i,j) \in P} O_i O_j O_i O_j,] where (\mathrm{sgn}(P) \in \pm 1)$ is the sign for pairing (P).
Our goal is to compute and interpret $(\mathrm{sgn}(P))$.
Our goal: derive the exact sign of each Wick contraction term.

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

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

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 $(-1)^{N_{\mathrm{swaps}}}$.

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_{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 $a^{\dagger}_{p_1} a_{q_1} a^{\dagger}_{p_2} a_{q_2} \cdots a^{\dagger}_{p_m} a_{q_m}$, 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:

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

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:

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

Grassmann Derivation (I)

Consider generating functional for Grassmann fields $\psi_p, \bar{\psi}_p$:

$$Z[\bar{\eta}, \eta] = \int \mathcal{D}(\bar{\psi}, \psi)\; e^{-\bar{\psi} G^{-1} \psi + \bar{\eta}\psi + \bar{\psi}\eta}.$$

Expanding the interaction

$$e^{-\bar{\psi} V \psi\psi} = \sum_n \frac{(-1)^n}{n!} (\bar{\psi}\bar{\psi}\psi\psi)^n$$

and performing Wick contractions via Gaussian integration generates all diagrams automatically.

Grassmann Derivation (II)

A closed fermion loop corresponds to a trace of propagators:

$$\mathrm{Tr}(GG\cdots G).$$

Under a cyclic permutation of Grassmann variables,

$$\psi_1\psi_2\cdots\psi_n = (-1)^{n-1}\psi_2\cdots\psi_n\psi_1.$$

Thus, each cyclic trace contributes a factor (-1) relative to bosons.
Hence:

$$\boxed{\text{Each closed fermion loop } \Rightarrow (-1).}$$

This reproduces the operator-based sign rule in a manifestly algebraic, field-theoretic way.

Summary of Fermionic Phase Rules

Goldstone Diagram Sign Rules

For any fermionic diagram in time-independent MBPT:

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

Each element contributes:

- Crossing of fermion lines: -1.
- Closed fermion loop: -1.
- Symmetry factor S from equivalent Wick contractions.

Final expression:

$$E^{(n)}_{\text{diagram}} = \frac{(-1)^{N_{\text{crossings}}+N_{\text{loops}}}}{S} \sum_{\text{indices}} \frac{\prod V_{\text{lines}}}{\Delta E_{\text{denominators}}}.$$

Hamiltonian Partition and Reference State

We consider

$$H = H_0 + V, \qquad H_0 |\Phi\rangle = E_0 |\Phi\rangle ,$$

with $|\Phi\rangle$ a Slater determinant (closed-shell, non-degenerate). Define projection operators

$$\mathcal{P} = |\Phi\rangle \langle\Phi| , \qquad \mathcal{Q} = 1 - \mathcal{P}.$$

Goal: Compute the exact ground-state energy E as an expansion in V centered at $|\Phi\rangle$.

RS Energy Expansion (Time-Independent MBPT)

Let $|\Psi\rangle$ be the exact ground state, normalized as $\langle\Phi|\Psi\rangle = 1$ (intermediate normalization). Then

$$E = E_0 + \Delta E, \qquad \Delta E = \sum_{n\geq 1} E^{(n)}.$$

Standard RS formulas (compactly):

$$E^{(1)} = \langle\Phi|V|\Phi\rangle, \qquad E^{(2)} = \sum_{\nu\neq 0} \frac{|\langle\Phi|V|\nu\rangle|^2}{E_0 - E_\nu^{(0)}}, \quad \ldots$$

Diagrammatically: each term $\leftrightarrow$ collection of Goldstone diagrams (closed, vacuum diagrams) built from V and H_0 lines/propagators.

Normal Ordering and Contractions (Assumed Known)

Write (w.r.t. $|\Phi\rangle$):

$$V =: V : + \underbrace{1a^{\dagger}1a}_{\text{contractions}} + \cdots$$

Wick's theorem (time-independent version) reduces expectation values to sums of products of contractions.

Diagram rules (Goldstone): vertices for V, lines for particle/hole propagators, symmetry factors S, energy denominators from ordered integrals / resolvents.

Vacuum-to-Vacuum Amplitude and Generating Picture

Introduce a bookkeeping parameter λ:

$$H(\lambda) = H_0 + \lambda V.$$

Define the (adiabatic) vacuum-to-vacuum amplitude

$$\mathcal{Z}(\lambda) \equiv \langle \Phi | \, \Omega(\lambda) \, | \Phi \rangle \, ,$$

where $\Omega(\lambda)$ denotes the Møller wave operator that maps $|\Phi\rangle$ to the interacting state in the adiabatic limit.

Heuristic: Many-body *vacuum diagrams* (closed diagrams) contribute to $\mathcal{Z}$. *Connected* vacuum diagrams contribute to $\log \mathcal{Z}$.

Statement: Linked Diagram (Linked-Cluster) Theorem

Theorem. *For time-independent MBPT with intermediate normalization, the ground-state energy correction ΔE 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 $\mathcal{Z}$ is the sum of all (linked and unlinked) vacuum diagrams,

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

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

Connected vs. Unlinked: A Visual Reminder

Connected   Unlinked (disconnected)

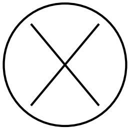
In algebra: products of lower-order *connected* contributions generate *unlinked* composites; these are precisely removed by the logarithm/normalization.

Goldstone Diagrams for Energy: Examples

Second order

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

(one connected bubble)

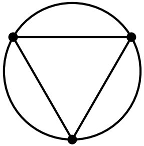


2nd order

Third order

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

(topologies: ring, ladder, crossed-ladder)



3rd order (ring)

Key Takeaways from Lecture 1

- Energies in RS-MBPT are sums over vacuum (closed) diagrams built from V.
- **Linked-Cluster Theorem:** only connected vacuum diagrams contribute to ΔE.
- The mechanism is combinatorial: unlinked diagrams exponentiate and cancel against normalization; $\log \mathcal{Z}$ generates connected clusters.

Next: formal derivation via cumulant (connected) expansion.

Derivation

1. Define the vacuum functional $\mathcal{Z}(\lambda)$ and its perturbative expansion
2. Show: $\log \mathcal{Z}(\lambda)$ collects only connected vacuum diagrams
3. Extract ΔE from $\log \mathcal{Z}$
4. Work through explicit 2nd and 3rd order to see cancellation of unlinked pieces

Vacuum Functional and Expansion

Introduce an adiabatic regulator (formal):

$$\mathcal{Z}(\lambda) = \frac{\langle\Phi|\,\Omega(\lambda)\,|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!}\,\langle\Phi|\,V^n\,|\Phi\rangle_{\text{connected+disconnected}}\,,$$

where Wick reduces $\langle\Phi|\,V^n\,|\Phi\rangle$ to sums of complete contractions.

Cluster decomposition: any complete contraction decomposes uniquely into a product of *connected* contractions (clusters).

Combinatorics of Clusters $\Rightarrow$ Exponentiation

Let C_n denote the sum of all connected vacuum contractions with n vertices of V. Then every disconnected contraction is a product of connected pieces:

$$\mathcal{Z}(\lambda) = 1 + \sum_{n\geq 1} \frac{\lambda^n}{n!}\Big(\text{all contractions}\Big) = \exp\left(\sum_{n\geq 1} \frac{\lambda^n}{n!}\, C_n\right).$$

Thus,

$$\boxed{\log \mathcal{Z}(\lambda) = \sum_{n\geq 1} \frac{\lambda^n}{n!}\, C_n \equiv \sum_{\text{connected vacuum diagrams}} .}$$

This is the *linked-cluster (connected) expansion*.

Extracting the Energy from $\log \mathcal{Z}$

With intermediate normalization ($\langle \Phi | \Psi \rangle = 1$) one can show

$$\Delta E = \frac{d}{d\lambda} \log \mathcal{Z}(\lambda) \bigg|_{\lambda=1}.$$

Expanded:

$$\Delta E = \sum_{n \geq 1} \frac{1}{n!} C_n,$$

where C_n are the n-th order *connected* (linked) vacuum diagrams evaluated with the usual Goldstone rules (including symmetry factors, energy denominators).

Sketch of the Proof (1): Wick and Cumulants

Idea: Write $\mathcal{Z} = \exp W$ with $W = \log \mathcal{Z}$, and interpret W as the *cumulant* generating functional of vacuum contractions.

- Introduce sources J linearly coupled to V or to field bilinears, expand $\mathcal{Z}[J]$.
- Cumulants (derivatives of $W[J]$ at $J = 0$) pick out *connected* correlation functions only.
- Setting J-structure to reproduce insertions of V yields C_n as the n-point connected vacuum objects.

This establishes $\log \mathcal{Z} = \sum$ connected non-constructively but generally.

Sketch of the Proof (2): Direct Counting

Alternatively, count how many times a product of connected pieces appears in $\mathcal{Z}$ vs. $\log \mathcal{Z}$:

$$\mathcal{Z} = \sum_{\{m_k\}} \prod_{k \geq 1} \frac{1}{m_k!} \left(\frac{C_k}{k!} \right)^{m_k},$$

where m_k is the multiplicity of k-vertex connected components and $\sum_k k\, m_k = n$ at n-th order.

$$\log \mathcal{Z} = \sum_{k \geq 1} \frac{C_k}{k!},$$

which follows from the exponential formula in combinatorics (the set-partition theorem). Hence only connected contributions survive in $\log \mathcal{Z}$.

Cancellation of Unlinked Diagrams in Energy

Energy from RS can also be written as

$$E = \frac{\langle \Phi | \, H \, | \Psi \rangle}{\langle \Phi | \Psi \rangle} = E_0 + \frac{\langle \Phi | \, V \, | \Psi \rangle}{\langle \Phi | \Psi \rangle}.$$

Expanding numerator and denominator in λ:

$$\frac{N(\lambda)}{D(\lambda)} = \frac{\sum_n \lambda^n N_n}{1 + \sum_{m \geq 1} \lambda^m D_m} = \sum_{r \geq 0} \lambda^r \Big(N_r - \sum_{m=1}^{r} D_m N_{r-m} + \cdots \Big),$$

and one finds precisely that terms factorizing into products of lower-order vacuum pieces cancel against the denominator. The survivors are the *linked* contributions, reproducing $\frac{\mathrm{d}}{\mathrm{d}\lambda} \log \mathcal{Z}$.

Goldstone Rules Refresher (for Energy Diagrams)

- Place n interaction vertices V; connect lines respecting fermionic statistics.
- Assign particle/hole propagators; each closed fermion loop $\Rightarrow$ a factor (-1).
- Symmetry factor S: divide by automorphisms that leave the diagram invariant.
- Energy denominator: product over intermediate-state energy differences (or via resolvent method).
- Sum over all internal indices (spin, orbitals); overall factor $1/n!$ from perturbative expansion cancels overcountings.

Explicit 2nd Order: Linked Only

For a two-body $V = \frac{1}{4} \sum \bar{v}_{pqrs} a_p^\dagger a_q^\dagger a_s a_r$,

$$E^{(2)} = \frac{1}{4} \sum_{ijab} \frac{\left|\bar{v}_{ijab}\right|^2}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b},$$

which corresponds to the single *connected* bubble diagram.

Any attempt to form products of first-order pieces is null because $E^{(1)}$ for normal-ordered V vanishes in a Hartree–Fock reference (or is absorbed in H_0), illustrating the absence/cancellation of unlinked composites at this order.

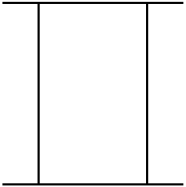
Explicit 3rd Order: Topologies and Cancellations

At third order, connected topologies include (schematically): ring, ladder, and crossed-ladder. Their analytical expressions (one example):

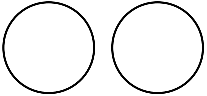
$$E^{(3)}_{\mathrm{lad}} = \frac{1}{8} \sum_{\substack{ijab \\ kc}} \frac{\bar{v}_{ijab}\, \bar{v}_{bkcj}\, \bar{v}_{cika}}{(\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b)(\varepsilon_i + \varepsilon_k - \varepsilon_a - \varepsilon_c)}.$$

Unlinked structures (products of a connected 2nd-order bubble with a disconnected 1st-order tadpole, etc.) cancel once the denominator normalization (or $\log \mathcal{Z}$) is accounted for.

Diagram Placeholders You Can Extend



Ladder (connected)



Unlinked (cancels)

Alternative Derivation Route: Bloch Equation

Let Ω be the wave operator, $|\Psi\rangle = \Omega\,|\Phi\rangle$, with the Bloch equation

$$[\Omega, H_0]\mathcal{P} = \mathcal{Q}(V\Omega - \Omega W)\mathcal{P}, \qquad W \equiv \mathcal{P}H\Omega\mathcal{P}.$$

Expanding $\Omega = \sum_{n\geq 0} \Omega^{(n)}$ and W order by order, one can show algebraically that the W (energy) receives only *connected* contributions, because the disconnected pieces generated in Ω cancel in W through $\mathcal{P}$-projection and the commutator structure. This is equivalent to the cumulant proof.

Summary of the Derivation

- Write the vacuum functional $\mathcal{Z}$ as a sum over all vacuum diagrams.
- Use cluster decomposition $\Rightarrow \mathcal{Z} = \exp\left(\sum \text{connected}\right)$.
- Take log and differentiate: $\Delta E = \frac{\mathrm{d}}{\mathrm{d}\lambda} \log \mathcal{Z}(\lambda)\big|_{\lambda=1}$.
- Hence ΔE equals the sum of values of *connected* vacuum diagrams only.

This holds to all orders and underpins size-extensivity and additivity for noninteracting fragments.

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).

Exercise

Task: For a two-body interaction in an HF basis, derive $E^{(3)}_{\text{ring}}$ explicitly:

1. Draw the connected ring topology and assign indices.
2. Write the algebraic expression using antisymmetrized matrix elements $\bar{v}_{pqrs}$.
3. Derive the energy denominators from intermediate-state energies.
4. Verify that any product of a 2nd-order connected and a 1st-order tadpole cancels in the normalized expression.

Take-Home Messages

- The linked (connected) nature of contributing diagrams to ΔE 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).