

The Linked Diagram Theorem in Time-Independent Many-Body Theory

MHJ, old notes

Roadmap: Two 45-minute Lectures

Lecture 1 (foundations)

- ▶ Setup: H_0 , V , reference $|\Phi\rangle$, projectors \mathcal{P} , \mathcal{Q}
- ▶ Rayleigh–Schrödinger (RS) MBPT and vacuum-to-vacuum amplitude
- ▶ Diagrammatics for ground-state energy corrections
- ▶ **Statement of the Linked Diagram (Linked-Cluster) Theorem**

Lecture 2 (derivation)

- ▶ Proof via cumulants / logarithm of the vacuum amplitude
- ▶ Cancellation of unlinked diagrams and normalization
- ▶ Explicit low-order examples (up to 3rd order)
- ▶ Practical notes: algorithmic generation and bookkeeping

Hamiltonian Partition and Reference State

We consider

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

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

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

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

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

Standard RS formulas (compactly):

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

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. $|\Phi\rangle$):

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

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.*

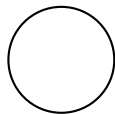
$$\Delta E = \sum_{\text{connected vacuum diagrams}} (\text{value of diagram})$$

Equivalently: if \mathcal{Z} is the sum of all (linked and unlinked) vacuum diagrams,

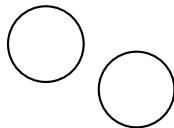
$$\log \mathcal{Z} = \sum_{\text{connected vacuum diagrams}},$$

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

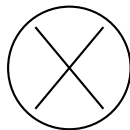
$$E^{(2)} = \sum_{\substack{ab \\ ij}} \frac{|\langle ij|V|ab\rangle|^2}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

(one connected bubble)

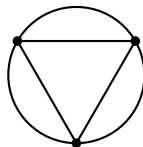
Third order

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

(topologies: ring, ladder, crossed-ladder)



2nd order



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.

Plan for Lecture 2

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):

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

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:

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

Thus,

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

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

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

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 :

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

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 $\frac{d}{d\lambda} \log \mathcal{Z}$.

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

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

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.

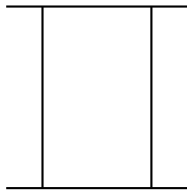
Explicit 3rd Order: Topologies and Cancellations

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

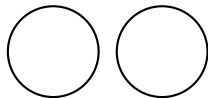
$$E_{\text{lad}}^{(3)} = \frac{1}{8} \sum_{\substack{ijab \\ kc}} \frac{\bar{v}_{ijab} \bar{v}_{bkcj} \bar{v}_{cika}}{(\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b)(\varepsilon_i + \varepsilon_k - \varepsilon_a - \varepsilon_c)}.$$

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

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

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 $\Rightarrow \mathcal{Z} = \exp(\sum \text{connected})$.
- ▶ Take log and differentiate: $\Delta E = \left. \frac{d}{d\lambda} \log \mathcal{Z}(\lambda) \right|_{\lambda=1}$.
- ▶ 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).

Worked Exercise (for Students)

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