

Green functions for open-shell systems

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Layout of the talk

- The quantum Graal
- The Gell-Mann and Low theorem
- The Green functions for open shells
- The generating function
- The Hopf algebra of derivations
- Non-perturbative equations
- The hierarchy of Green functions
- The hierarchy of connected Green functions
- Open questions
- Conclusions

The quantum Graal

- $H|\Psi\rangle = E|\Psi\rangle$
- H is the nonrelativistic Hamiltonian

$$H = - \sum_{i=1}^N \frac{\hbar^2 \Delta_i}{2m} + \sum_{i=1}^N V_n(\mathbf{r}_i) + \sum_{i \neq j} V_c(|\mathbf{r}_i - \mathbf{r}_j|)$$

- Density $n(\mathbf{r}) = \sum_i \langle \Psi | \delta(\mathbf{r} - \mathbf{r}_i) | \Psi \rangle$.
- Atoms or small molecules: direct diagonalization
- Solids: Density functional theory
- Solids: Green functions with non-perturbative approximations (GW approximation, Bethe-Salpeter equation)

The Gell-Mann and Low theorem

- Perturbation theory $H = H_0 + H_1$

$$H_0 = - \sum_{i=1}^N \frac{\Delta_i}{2m} + \sum_{i=1}^N V_n(\mathbf{r}_i), \quad H_1 = \sum_{i \neq j} V_c(|\mathbf{r}_i - \mathbf{r}_j|)$$

- Adiabatic switching $H(\epsilon t) = H_0 + f(\epsilon t)H_1$
- Interaction picture $H^{\text{int}}(t) = f(\epsilon t)e^{iH_0 t} H_1 e^{-iH_0 t}$
- Evolution operator

$$U(t, t') = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int dt_1 \dots dt_n T(H^{\text{int}}(t_1) \dots H^{\text{int}}(t_n))$$

- If $|\Phi_0\rangle$ is the non-degenerate ground state of H_0 :

$$|\Psi_{\text{GL}}\rangle = \lim_{\epsilon \rightarrow 0} \frac{U(0, -\infty)|\Phi_0\rangle}{\langle \Phi_0 | U(0, -\infty) | \Phi_0 \rangle}$$
 is an eigenstate of H

- Proof by Nenciu and Rasche (Helv. Phys. Acta **62** (1989) p.372-88) if f , f' and f'' are in L^1 and if H_0 and H_1 are self-adjoint, H_0 is bounded from below and H_1 is bounded with respect to H_0 : for $|\psi\rangle$ in the domain of H_0 ,
 $\|H_1|\psi\rangle\| \leq a\|H_0|\psi\rangle\| + b\||\psi\rangle\|$ with $a < 1$.

The Gell-Mann and Low theorem: discussion

- $|\Psi_{\text{GL}}\rangle$ is an eigenstate of H but not necessarily the *ground* state of H .
- Rule of thumb: The Gell-Mann and Low state is the ground state of the interacting system if the energy difference between the ground state and the first excited state of the non-interacting system is large compared with the interaction energy.
- This condition rarely satisfied in practice
- The Gell-Mann and Low theorem is not valid for degenerate or quasi-degenerate non-interacting systems
- The standard Green function (i.e. many-body) theory does not work for open shell systems.

Solution: Green functions for open shells

- Start from a set of low-energy states $|i\rangle$ of the non-interacting system
- Transform them into states of the interacting system by $|\Psi_i\rangle = U(0, -\infty)|i\rangle$

- Calculate the energy matrix of the interacting system

$$H_{ij} = \langle i|U(+\infty, 0)(H_0 + H^{\text{int}}(0))U(0, -\infty)|j\rangle$$

- Diagonalize it
- The matrix to diagonalize is very small (it contains only the lowest energy states of the non-interacting system)
- Powerful non-perturbative methods of the Green function theory can be used to calculate H_{ij} .
- Describes the degeneracy splitting due to the interaction

Green functions for open shells: density matrix

- Start from a density matrix $\hat{\rho} = \sum_{ij} \rho_{ij} |i\rangle \langle j|$ of the non-interacting system
- Calculate the energy $E(\rho)$ of the interacting system
- Minimize $E(\rho)$ with respect to ρ
- Preserves the symmetry of the system
- Green functions
 - Self-consistent determination of the orbitals
 - Resummation of infinite families of terms of the perturbative expansion
 - Detailed description of the electron-hole interactions through the Bethe-Salpeter equation
 - Beyond the coupled-cluster method
- The many-body theory is recovered for closed shells
- The crystal field equations are recovered as the first term of the perturbative expansion of the equations for the Green functions for open shells

The Green functions

- One-body operators

$$\langle f \rangle = \sum_{mn} \rho_{nm} \langle \Psi_m | \sum_i f(\mathbf{r}_i) | \Psi_n \rangle = \sum_i \text{tr}(\hat{\rho} f(\mathbf{r}_i)).$$

- Examples

- The electron density $\langle n(\mathbf{r}) \rangle = \sum_i \text{tr}(\hat{\rho} \delta(\mathbf{r} - \mathbf{r}_i))$.
- The velocity $\langle \mathbf{v} \rangle = \sum_i \text{tr}(\hat{\rho} \nabla_i)$.

- The one-body Green function $G(x, y)$ with $x = (\mathbf{r}, t)$ is such that, for any one-body operator f

$$\langle f \rangle = -\frac{1}{\pi} \int \Im(G(x, x)) f(\mathbf{r}) d\mathbf{r}$$

- Two-body operators (Coulomb energy, dielectric function)

$$\langle g \rangle = \sum_{ij} \text{tr}(\hat{\rho} g(\mathbf{r}_i, \mathbf{r}_j)).$$

- The expectation value of two-body operators can be calculated from the two-body Green function

$$G_2(x_1, x_2, y_1, y_2)$$

The generating function for the Green functions

- There is a function $Z(j)$, with $j = (j_+, j_-)$, that generates all the Green functions. For example

$$G(x, y) = (-i)^2 \frac{Z(j)}{\delta j(x) \delta j(y)} \Big|_{j_+ = j_- = 0}.$$

- $A(\varphi)$ is the interacting Hamiltonian

$$A(\varphi) = \frac{e^2}{8\pi\epsilon_0} \int \frac{\bar{\varphi}(x) \bar{\varphi}(x') \delta(t - t') \varphi(x') \varphi(x)}{|\mathbf{r} - \mathbf{r}'|} dx dx'$$

- $Z(j) = e^{-iD} Z_0(j)$ with $D = A\left(\frac{\delta}{i\delta j_+}\right) - A\left(\frac{\delta}{i\delta j_-}\right)$

and $Z_0(j) = e^{W_0(j)}$ with

$$W_0(j) = -\frac{1}{2} \int j(x) G^0(x, y) j(y) + K_\rho(j_+ + j_-)$$

$$K_\rho(k) = \log \left(\text{tr}(\hat{\rho} : e^{i \int dx \varphi(x) k(x)} :) \right)$$

- Cumulants of $\hat{\rho}$ (initial correlations)

$$K_\rho(k) = \int dx_1 dy_1 K_\rho^{(1)}(x_1, y_1) k(x_1) k(y_1) + \int dx dy K_\rho^{(2)}(x_1, x_2, y_1, y_2) k(x_1) k(x_2) k(y_1) k(y_2) + \dots$$

Correlation as propagators

- One-body correlation function

$$K_{\rho}^{(1)}(x, y) = \sum_{ij} \rho_{ij} \langle j | : \psi(x) \psi^{\dagger}(y) : | i \rangle = \begin{array}{c} \bullet \text{---} \bullet \\ x \qquad y \end{array}$$

- One-body propagator: $G_{\rho}^0 = G^0 + K_{\rho}^{(1)}$.

- Two-body correlation function

$$\sum_{ij} \rho_{ij} \langle j | : \psi^{\dagger}(x_1) \psi^{\dagger}(x_2) \psi(y_2) \psi(y_1) : | i \rangle = \begin{array}{c} \bullet \text{---} \bullet \\ x_1 \qquad y_1 \\ \bullet \text{---} \bullet \\ x_2 \qquad y_2 \end{array} + \begin{array}{c} \bullet \text{---} \bullet \\ x_1 \qquad y_1 \\ \bullet \text{---} \bullet \\ x_2 \qquad y_2 \end{array} + \begin{array}{c} \bullet \text{---} \bullet \\ x_1 \qquad y_1 \\ \bullet \text{---} \bullet \\ x_2 \qquad y_2 \end{array} \\ K_{\rho}^{(2)}$$

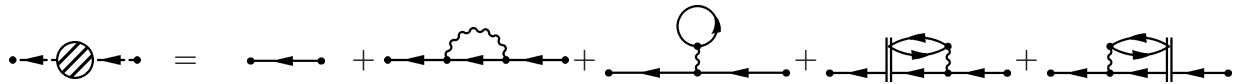
- Two-body propagator: $K_{\rho}^{(2)}(x_1, x_2, y_1, y_2)$
 - it is zero for a single Slater determinant $|i\rangle$
 - it is the source of the multiplets
- Three body propagator

$$K_{\rho}^{(3)}(x_1, x_2, x_3, y_1, y_2, y_3) = \begin{array}{c} \bullet \text{---} \bullet \\ x_1 \qquad y_1 \\ \bullet \text{---} \bullet \\ x_2 \qquad y_2 \\ \bullet \text{---} \bullet \\ x_3 \qquad y_3 \end{array}$$

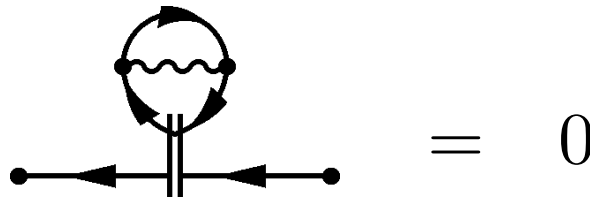
- beyond the multiplets
- For a M -fold degenerate system, up to M -body propagators

Perturbative expansion

- Green function $G(x, y) = -Z^{-1} \delta_{j(y)} \delta_{j(y)} Z$
- Use $Z = e^{-iD} Z_0$ and expand the exponential



- Cancellation theorems



- Early history
 - Schwinger 1960
 - Kadanoff Baym 1962
 - Keldysh 1965
- Assuming $K_\rho^{(n)} = 0$ for $n > 1$: around 1000 papers
- Keeping all $K_\rho^{(n)}$: 4 papers, 49 pages
 - Fujita 1969
 - Hall 1975
 - Tikhodeev and Kukharenko 1982

The Hopf algebra of derivations

The algebra

- \mathcal{A} : algebra of differential operators with constant coefficients
- Generators of \mathcal{A} : partial derivatives $\partial_i = \frac{\partial}{\partial x_i}$,
- Basis of \mathcal{A} : multiple partial derivatives $\frac{\partial^n}{\partial x_{i_1} \dots \partial x_{i_n}}$ for $n \geq 1$.
- Product: derivatives of derivatives $\partial_i \partial_j = \frac{\partial^2}{\partial x_i \partial x_j}$
- Unit $\mathbf{1}$: for any $D \in \mathcal{A}$, $D\mathbf{1} = \mathbf{1}D = D$.
- Example: $\frac{1}{\sqrt{2}}\mathbf{1} + \frac{\partial}{\partial x_1} - 4\frac{\partial^2}{\partial x_2 \partial x_3} \in \mathcal{A}$.
- \mathcal{A} with the product of derivations is a unital associative algebra.

The Hopf algebra of derivations

The coproduct

- Action of the derivations on functions

$$\mathbf{1}(fg) = fg.$$

$$\partial_i(fg) = (\partial_i f)g + f(\partial_i g). \quad (\text{Leibniz})$$

$$\begin{aligned} \partial_i \partial_j(fg) &= (\partial_i \partial_j f)g + (\partial_i f)(\partial_j g) + \\ &\quad (\partial_j f)(\partial_i g) + f(\partial_i \partial_j g). \end{aligned}$$

- $D(fg) = \sum (D_{(1)} f)(D_{(2)} g).$
- $\Delta : \mathcal{A} \rightarrow \mathcal{A} \otimes \mathcal{A}, \quad \Delta D = \sum D_{(1)} \otimes D_{(2)}.$
- Coproduct

$$\Delta \mathbf{1} = \mathbf{1} \otimes \mathbf{1}.$$

$$\Delta \partial_i = \partial_i \otimes \mathbf{1} + \mathbf{1} \otimes \partial_i.$$

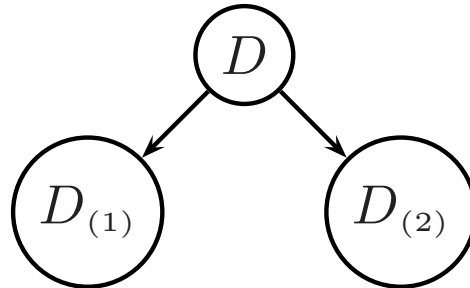
$$\Delta \partial_i \partial_j = \partial_i \partial_j \otimes \mathbf{1} + \partial_i \otimes \partial_j + \partial_j \otimes \partial_i + \mathbf{1} \otimes \partial_i \partial_j.$$

- $\Delta(DD') = (\Delta D)(\Delta D')$

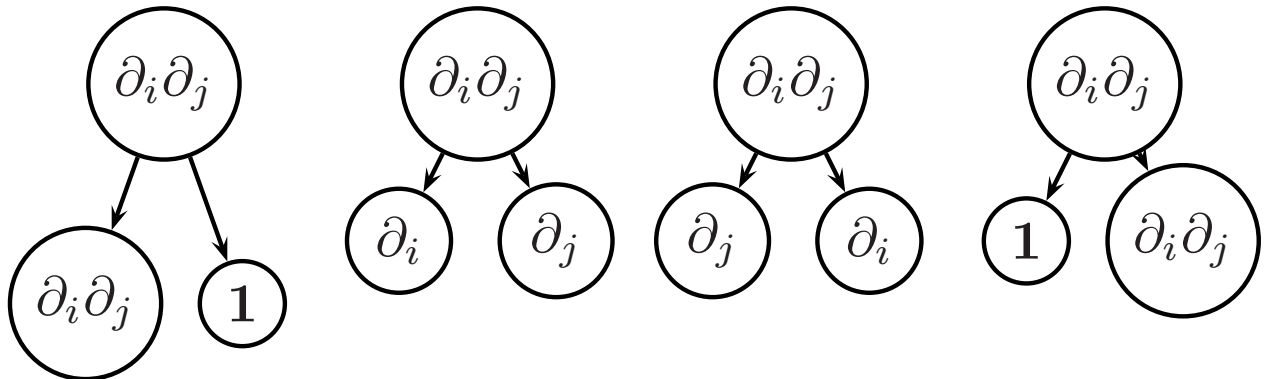
$$\Delta(\partial_i \partial_j) = (\partial_i \otimes \mathbf{1} + \mathbf{1} \otimes \partial_i)(\partial_j \otimes \mathbf{1} + \mathbf{1} \otimes \partial_j).$$

Coproduct: splitting into two parts

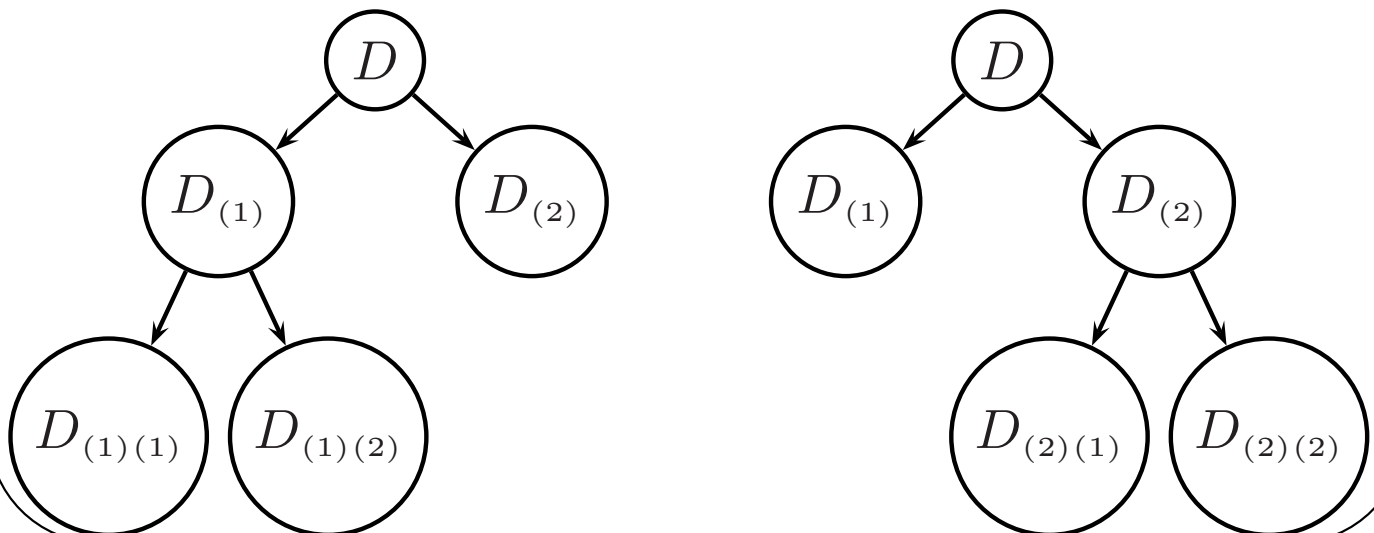
$$\Delta D = \sum D_{(1)} \otimes D_{(2)}$$



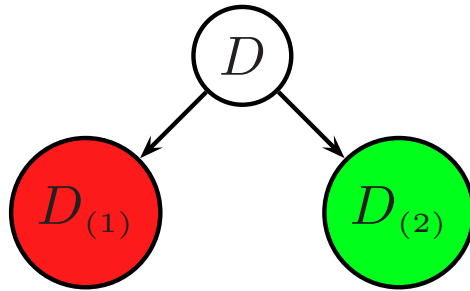
$$\Delta(\partial_i \partial_j) = \partial_i \partial_j \otimes \mathbf{1} + \partial_i \otimes \partial_j + \partial_j \otimes \partial_i + \mathbf{1} \otimes \partial_i \partial_j$$



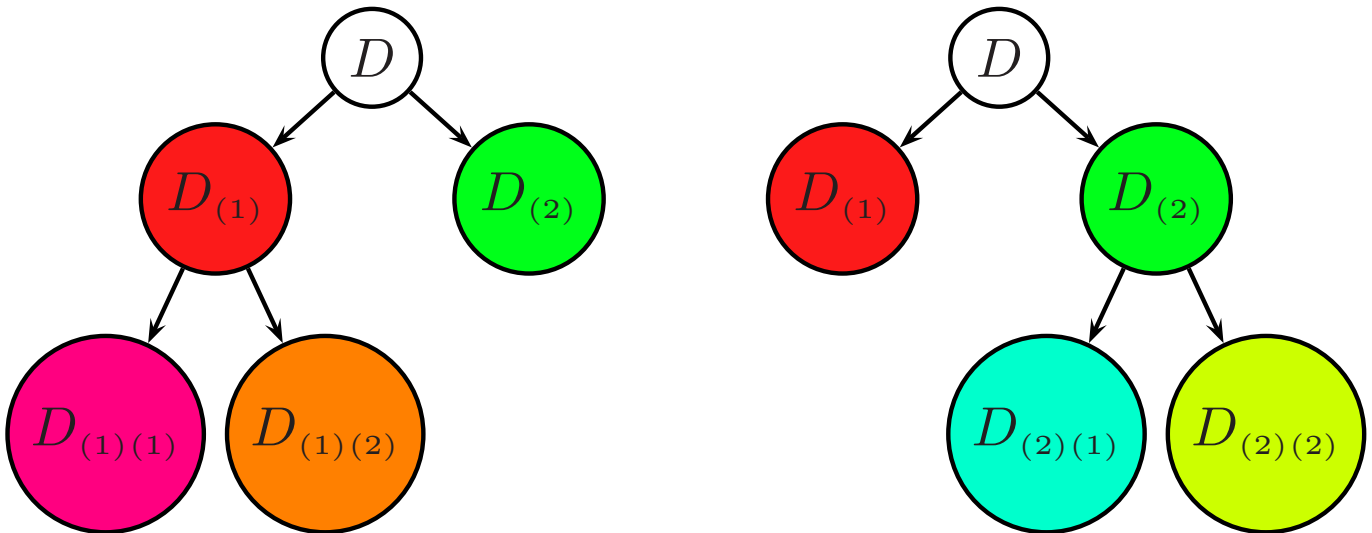
Splitting into three parts?



Coassociativity

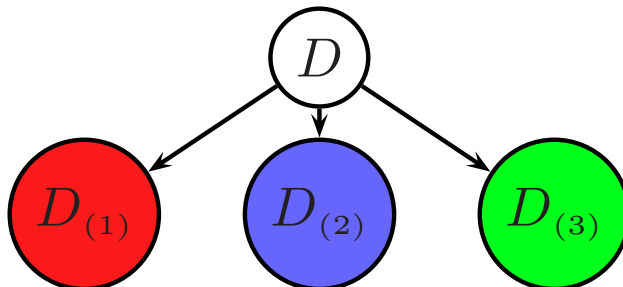


$$\Delta D = \sum D_{(1)} \otimes D_{(2)}$$



$$\sum (\Delta D_{(1)}) \otimes D_{(2)} = \sum D_{(1)} \otimes (\Delta D_{(2)})$$

$$(\Delta \otimes \text{Id})\Delta D = (\text{Id} \otimes \Delta)\Delta D = \sum D_{(1)} \otimes D_{(2)} \otimes D_{(3)}$$



The Hopf algebra of derivations

Coassociativity

- $D(fg) = \sum (D_{(1)}f)(D_{(2)}g)$.
- $fgh = fg h = f gh$.
- $D(fgh) = \sum (D_{(1)}(fg))(D_{(2)}h) = \sum (D_{(1)}f)(D_{(2)}(gh))$
 $= \sum (D_{(1)}f)(D_{(2)}g)(D_{(3)}h)$.
- $(\Delta \otimes \text{Id})\Delta D = (\text{Id} \otimes \Delta)\Delta D = \sum D_{(1)} \otimes D_{(2)} \otimes D_{(3)}$.
- Example $\Delta \partial_i = \partial_i \otimes \mathbf{1} + \mathbf{1} \otimes \partial_i$.
 $(\Delta \otimes \text{Id})\Delta \partial_i = (\Delta \partial_i) \otimes \mathbf{1} + (\Delta \mathbf{1}) \otimes \partial_i$
 $= \partial_i \otimes \mathbf{1} \otimes \mathbf{1} + \mathbf{1} \otimes \partial_i \otimes \mathbf{1} + \mathbf{1} \otimes \mathbf{1} \otimes \partial_i$.
 $(\text{Id} \otimes \Delta)\Delta \partial_i = \partial_i \otimes (\Delta \mathbf{1}) + \mathbf{1} \otimes (\Delta \partial_i)$
 $= \partial_i \otimes \mathbf{1} \otimes \mathbf{1} + \mathbf{1} \otimes \partial_i \otimes \mathbf{1} + \mathbf{1} \otimes \mathbf{1} \otimes \partial_i$.
- $D(f_1 \dots f_n) = \sum (D_{(1)}f_1) \dots (D_{(n)}f_n)$.

Second step of the calculation of $Z(j)$

- We want to calculate

$$Z = e^{-iD} Z_0.$$

- We put $Z_0 = e^{W_0}$ with

$$W_0 = -\frac{1}{2} \int j(x) G^0(x, y) j(y) + K_\rho(j_+ + j_-)$$

– K_ρ is the generating function of the cumulants of $\hat{\rho}$

- We take the functional derivative with respect to $j(x)$

$$\frac{\delta Z}{\delta j(x)} = e^{-iD} \frac{\delta Z_0}{\delta j(x)} = e^{-iD} \left(\frac{\delta W_0}{\delta j(x)} Z_0 \right).$$

- Coproduct

$$\frac{\delta Z}{\delta j(x)} = \sum \left((e^{-iD})_{(1)} \frac{\delta W_0}{\delta j(x)} \right) \left((e^{-iD})_{(2)} Z_0 \right).$$

- How to calculate Δe^{-iD} ?

Resummation of Δe^{-iD}

- Perturbative formula

$$\begin{aligned}\Delta e^{-iD} &= 1 \otimes 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \Delta D^n \\ &= 1 \otimes 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} D_{(1)}^n \otimes D_{(2)}^n\end{aligned}$$

- Problem ΔD^n contains the term $1 \otimes D^n$ so that Δe^{-iD} is an infinite series
- Reduced coproduct with respect to D :

$$\begin{aligned}\Delta' D &= \Delta D - 1 \otimes D - D \otimes 1 \\ &= \sum D_{(1')} \otimes D_{(2')}, \\ \Delta'(D^{n+1}) &= \sum D_{(1')}^n D_{(1')} \otimes D_{(2')}^n D_{(2')}.\end{aligned}$$

- Examples:

- If $D = \delta_j$ then $\Delta' D^n = 0$
- If $D = \delta_j^2$ then $\Delta' D^n = 2^n \delta_j^n \otimes \delta_j^n$

- The degree of $D_{(1')}^n$ and $D_{(2')}^n$ is at least n

Resummation of Δe^{-iD}

- Main identity

$$\Delta(D^n) = \sum_{i+j+k=n} \frac{n!}{i!j!k!} D_{(1')}^i D^j \otimes D_{(2')}^i D^k.$$

- Consequence (for any commutative Hopf algebra and any D of degree > 0)

$$\begin{aligned} \Delta e^D &= \sum_{n=0}^{\infty} \frac{1}{n!} D_{(1')}^n e^D \otimes D_{(2')}^n e^D \\ &= (\Delta' e^D)(e^D \otimes e^D). \end{aligned}$$

- Generating function

$$\begin{aligned} \frac{\delta Z}{\delta j(x)} &= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \sum \left(D_{(1')}^n e^{-iD} \frac{\delta W_0}{\delta j(x)} \right) \\ &\quad \left(D_{(2')}^n e^{-iD} Z_0 \right) \\ &= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \sum \left(D_{(1')}^n \frac{\delta W_1}{\delta j(x)} \right) \left(D_{(2')}^n Z \right) \end{aligned}$$

with $W_1 = e^{-iD} W_0$

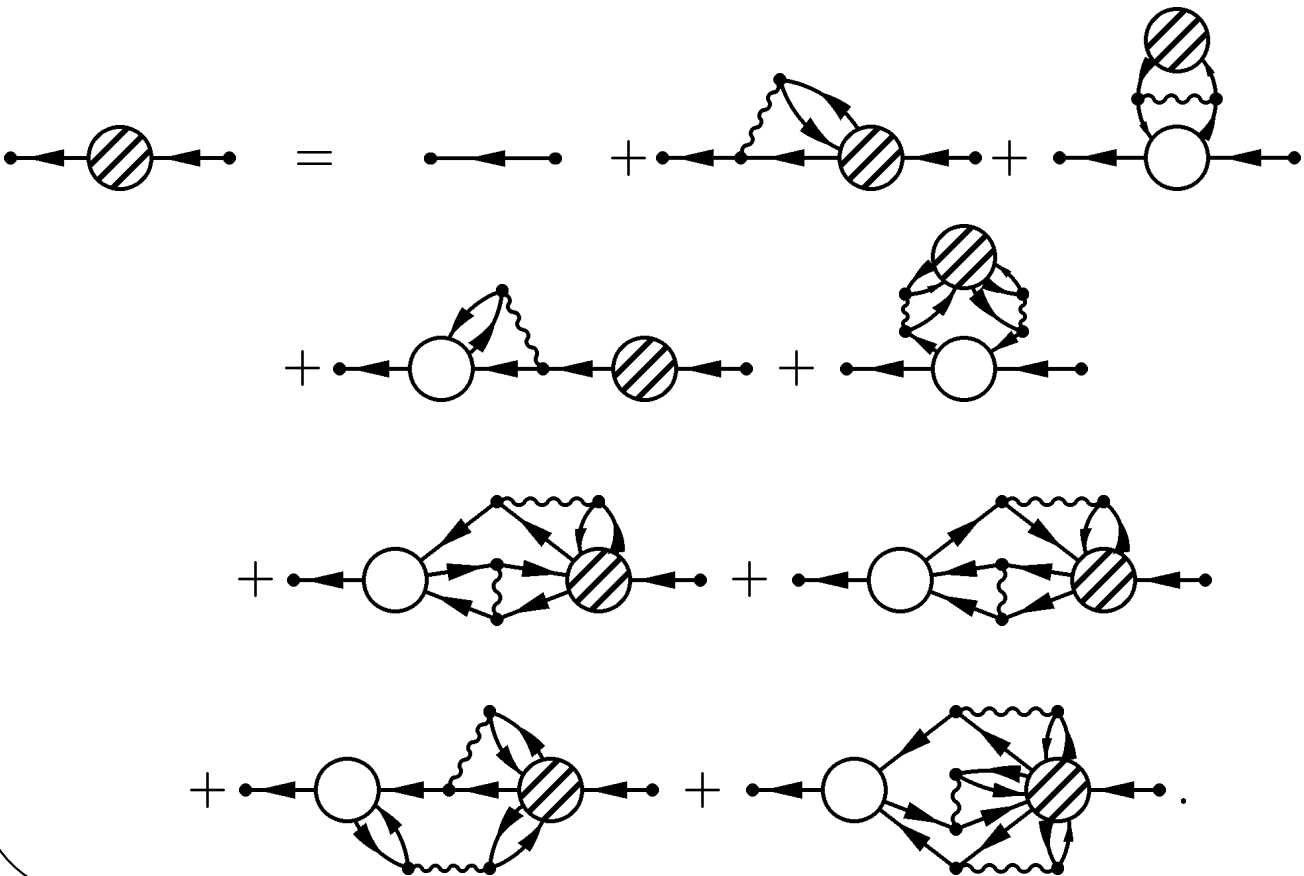
- The sum is now finite

Hierarchy of Green functions

- Green function

$$\begin{aligned}
 G(x, y) &= - \frac{\delta^2 Z}{\delta j(x) \delta j(y)} \Big|_{j=0} = \\
 &= - \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \sum \left(D_{(1')}^n \frac{\delta^2 W_1}{\delta j(x) \delta j(y)} \right) \left(D_{(2')}^n Z \right) \\
 &= - \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \sum \left(D_{(1')}^n \frac{\delta W_1}{\delta j(x)} \right) \left(D_{(2')}^n \frac{\delta Z}{\delta j(y)} \right)
 \end{aligned}$$

- In diagrams, for K_ρ of degree 4



Hierarchy of connected Green functions

- The connected Green functions are generated by $W = \log Z$

- The reduced coproduct

$$\underline{\Delta}d = \Delta d - 1 \otimes d - d \otimes 1$$

- Main identity: if the degree of d is > 0

$$d(u^n) = \sum_{k=1}^n \binom{n}{k} u^{n-k} \sum d_{(\underline{1})} u \dots d_{(\underline{k})} u,$$

- Consequence: if $f(z)$ is analytic

$$d(f(u)) = \sum_{k=1}^{\infty} \frac{f^{(k)}(u)}{k!} \sum d_{(\underline{1})} u \dots d_{(\underline{k})} u,$$

- In particular

$$d(e^u) = e^u \sum_{k=1}^{\infty} \frac{1}{k!} \sum d_{(\underline{1})} u \dots d_{(\underline{k})} u.$$

Hierarchy of connected Green functions

- We define W by $Z = e^W$
- We rewrite

$$\frac{\delta e^W}{\delta j(x)} = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \sum \left(D_{(1')}^n \frac{\delta W_1}{\delta j(x)} \right) \left(D_{(2')}^n e^W \right)$$

- For connected Green functions

$$\begin{aligned} \frac{\delta W}{\delta j(x)} &= \frac{1}{Z} \frac{\delta Z}{\delta j(x)} \\ &= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \sum_{k=1}^{\infty} \frac{1}{k!} \sum \left(D_{(1')}^n \frac{\delta W_1}{\delta j(x)} \right) \\ &\quad \left(D_{(2')(\underline{1})}^n W \right) \dots \left(D_{(2')(\underline{k})}^n W \right). \end{aligned}$$

- The sum is finite because the degree of each $D_{(2')(\underline{i})}^n$ is greater than zero and their sum is the degree of $D_{(2')}^n$, which is finite

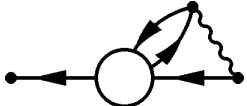
What is yet to be done

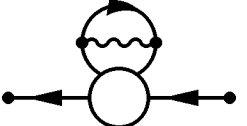
- Determine the structure of the Green functions
- Write Green functions in terms of one-particle irreducible vertices
- For the one-body Green function G
 - Closed shells $G = G^0 + G^0 \Sigma G$
 - Open shells (Hall 1974)

$$G = \overleftarrow{M}(G^0 + \overleftrightarrow{\Sigma})\overrightarrow{M}(1 + \Sigma G)$$

with

$$\overleftarrow{M} = 1 + \sum_{n=1}^{\infty} (\overleftarrow{\Sigma})^n \quad \text{and} \quad \overrightarrow{M} = 1 + \sum_{n=1}^{\infty} (\overrightarrow{\Sigma})^n.$$

$$\overleftarrow{\Sigma} = \text{Diagram 1} + \dots$$


$$\overrightarrow{\Sigma} = \text{Diagram 2} + \dots$$


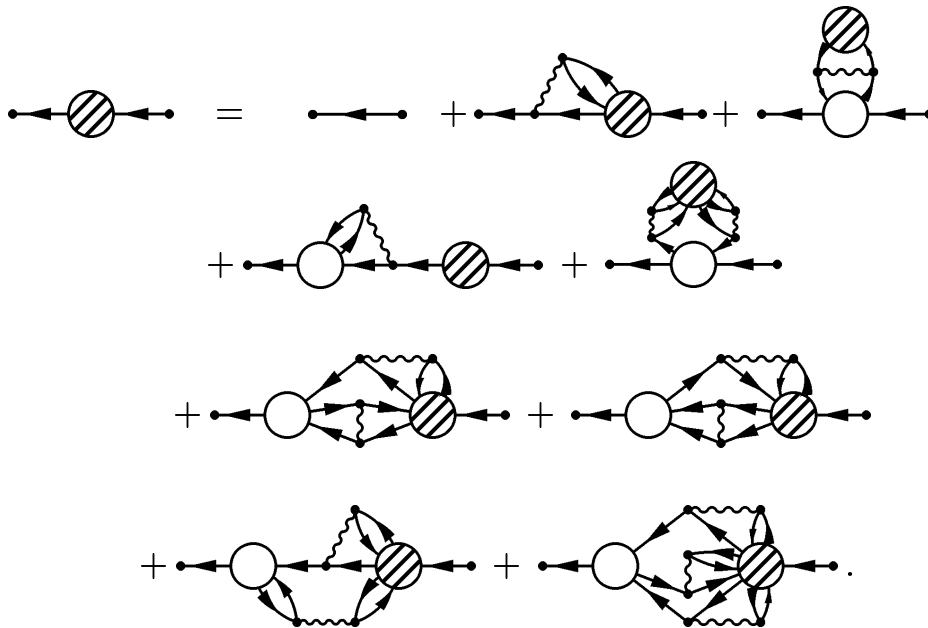
- Closed shells: $\overleftarrow{\Sigma} = \overrightarrow{\Sigma} = \overleftrightarrow{\Sigma} = 0$

The self-energy: source of the problem

- $(i\partial_t - H_0)G^0 = 1$
- Closed shell case:

$$G = G^0 + G^0 \Sigma G \Leftrightarrow (i\partial_t - H_0)G = 1 + \Sigma G$$

- But $(i\partial_t - H_0)f = 0$ has solutions
- Hierarchy for G :



- $(i\partial_t - H_0)G$ kills all the terms except for the first two because

$$(i\partial_t - H_0) \frac{\delta K_\rho}{\delta j} = 0.$$

Signs of hope

- Define auxiliary Green functions

$$\vec{\bar{G}} = (1 + G\Sigma)\overleftarrow{\bar{M}}$$

$$\overleftarrow{\bar{G}} = \vec{\bar{M}}(1 + \Sigma G)$$

$$\overleftarrow{\bar{G}} = \vec{\bar{M}}(\Sigma + \Sigma G\Sigma)\overleftarrow{\bar{M}}$$

- The Hall equation becomes $\bar{G} = \bar{G}^0 + \bar{G}^0\bar{\Sigma}\bar{G}$,

with

$$\bar{G}^0 = \begin{pmatrix} G^0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\bar{G} = \begin{pmatrix} G & \overrightarrow{G} \\ \overleftarrow{G} & \overleftarrow{G} \end{pmatrix},$$

$$\bar{\Sigma} = \begin{pmatrix} \Sigma & \overrightarrow{\Sigma} \\ \overleftarrow{\Sigma} & \overleftarrow{\Sigma} \end{pmatrix}$$

- \bar{G}^0 is now invertible

The Bethe-Salpeter equation

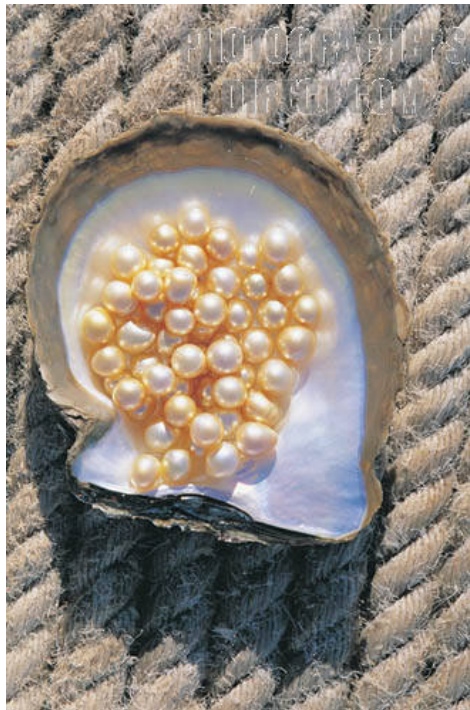
- Two-body Green function $G_2(x_1, x_2, y_1, y_2)$
- Closed shells $G_2 = G_1 G_1 + G_1 G_1 K G_2$
- K is a two-particle irreducible kernel
- Open shells ?
- Legendre transforms ?

Conclusion

- The closed-shell case is well mastered



- The open-shell case might reveal some pearls



The method of generating functions

- $A = \int_{-\infty}^{\infty} H^{\text{int}}(t) dt$
- $A = \int dx V(\varphi(x))$ with $x = (t, \mathbf{r})$
- In fact

$$A = \frac{e^2}{8\pi\epsilon_0} \int \frac{\bar{\varphi}(x)\bar{\varphi}(x')\delta(t-t')\varphi(x')\varphi(x)}{|\mathbf{r}-\mathbf{r}'|} dx dx'$$

- The S-matrix is

$$S = U(-\infty, \infty) = T(e^{-iA}).$$

- Generating function

$$\begin{aligned} S(j) &= T(e^{-iA+i \int dx \varphi(x)j(x)}) \\ &= \exp\left(-iA\left(\frac{-i\delta}{\delta j(x)}\right)\right) T(e^{i \int dx \varphi(x)j(x)}). \end{aligned}$$

The generating function for the Green functions

- The one-body Green function $G(x, y)$

$$G(x, y) = \text{tr}(\hat{\rho} S^\dagger(j) T(\phi(x)\phi(y)S(j)))|_{j=0}.$$

- Doubling of sources

$$Z(j_+, j_-) = \text{tr}(\hat{\rho} S^\dagger(j_-) S(j_+)).$$

- Generates the Green functions

$$G(x, y) = (-i)^2 \frac{Z(j_+, j_-)}{\delta j_+(x) \delta j_+(y)}|_{j_+=j_-=0}.$$

- Calculation of the generating function, $j = (j_+, j_-)$

$$Z(j) = \exp\left(-iA\left(\frac{-i\delta}{\delta j_+(x)}\right) + iA\left(\frac{-i\delta}{\delta j_-(x)}\right)\right) \text{tr}\left(\hat{\rho} \bar{T}\left(e^{i \int dx \varphi(x) j_-(x)}\right) T\left(e^{i \int dx \varphi(x) j_+(x)}\right)\right)$$

First step of the calculation of $Z(j)$

- We want to calculate

$$Z(j) = \exp \left(-iA \left(\frac{-i\delta}{\delta j_+(x)} \right) + iA \left(\frac{-i\delta}{\delta j_-(x)} \right) \right) \text{tr} \left(\hat{\rho} \bar{T} \left(e^{i \int dx \varphi(x) j_-(x)} \right) T \left(e^{i \int dx \varphi(x) j_+(x)} \right) \right)$$

- Compute the trace

$$\begin{aligned} Z_0(j) &= \text{tr} \left(\hat{\rho} \bar{T} \left(e^{i \int dx \varphi(x) j_-(x)} \right) T \left(e^{i \int dx \varphi(x) j_+(x)} \right) \right) \\ &= e^{-\frac{1}{2} \int j(x) G^0(x,y) j(y) + K_\rho(j_+ + j_-)} \end{aligned}$$

with $K_\rho(j_+ + j_-) = \log \left(\text{tr} \left(\hat{\rho} : e^{i \int dx \varphi(x) (j_+(x) + j_-(x))} : \right) \right)$

- Define the differential operator

$$D = A \left(\frac{-i\delta}{\delta j_+(x)} \right) - A \left(\frac{-i\delta}{\delta j_-(x)} \right)$$

- The generating function becomes

$$Z(j) = e^{-iD} Z_0(j).$$