Green functions for open-shell systems

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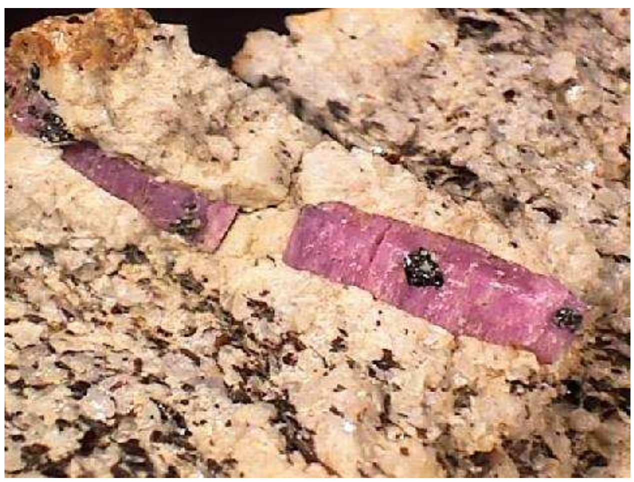


Layout of the talk

- 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 $H^{\mathrm{int}}(t) = f(\epsilon t) \mathrm{e}^{iH_0 t} H_1 \mathrm{e}^{-iH_0 t}$
- Evolution operator

$$U(t, t') = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int \mathrm{d}t_1 \ldots \mathrm{d}t_n T\big(H^{\mathrm{int}}(t_1) \ldots H^{\mathrm{int}}(t_n)\big)$$

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

$$|\Psi_{\mathrm{GL}}\rangle = \lim_{\epsilon \to 0} \frac{U(0, -\infty)|\Phi_0\rangle}{\langle \Phi_0 | U(0, -\infty) | \Phi_0 \rangle}$$ 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

- $|\Psi_{\mathrm{GL}}\rangle$ 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 excitated 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

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

- 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

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

- Examples
  - The electron density $\langle n(\mathbf{r}) \rangle = \sum_i \mathrm{tr}\big(\hat{\rho}\delta(\mathbf{r} - \mathbf{r}_i)\big)$.
  - The velocity $\langle \mathbf{v} \rangle = \sum_i \mathrm{tr}\big(\hat{\rho}\nabla_i\big)$.
- The one-body Green function $G(x, y)$ with $x = (\mathbf{r}, t)$ is such that, for any one-body operator f

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

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

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

- 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

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

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

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

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

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

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

$$K_\rho(k) \quad = \quad \log\Big(\mathrm{tr}\big(\hat{\rho}{:}\mathrm{e}^{i\int \mathrm{d}x \varphi(x) k(x)}{:}\big)\Big)$$

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

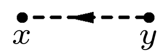
$$K_\rho(k) \quad = \quad \int \mathrm{d}x_1 \mathrm{d}y_1 K_\rho^{(1)}(x_1,y_1) k(x_1) k(y_1) +$$

$$\int \mathrm{d}x \mathrm{d}y K_\rho^{(2)}(x_1,x_2,y_1,y_2) k(x_1) k(x_2) k(y_1) k(y_2) + \dots$$

Correlation as propagators

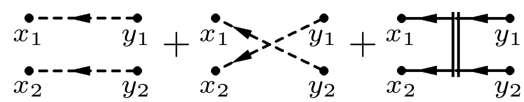
- One-body correlation function

$$K_\rho^{(1)}(x,y) \quad = \quad \sum_{ij} \rho_{ij} \langle j| {:}\psi(x)\psi^\dagger(y){:} |i\rangle =$$



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

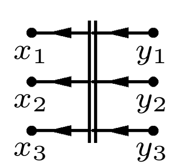
$$\sum_{ij} \rho_{ij} \langle j| {:}\psi^\dagger(x_1)\psi^\dagger(x_2)\psi(y_2)\psi(y_1){:} |i\rangle \quad =$$



$K_\rho^{(2)}$

- 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

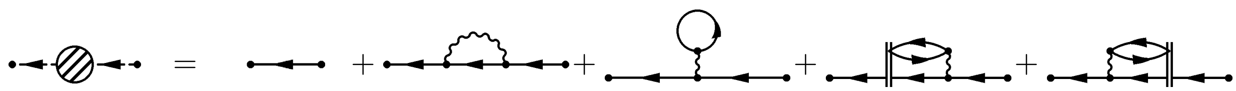
$$K_\rho^{(3)}(x_1, x_2, x_3, y_1, y_2, y_3) \quad =$$



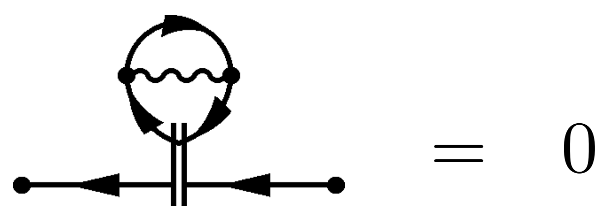
  - beyond the multiplets
- For a M-fold degenerate system, up to M-body propagators

Perturbative expansion

- Green function $G(x,y) = -Z^{-1}\delta_{j(y)}\delta_{j(y)}Z$
- Use $Z = \mathrm{e}^{-iD}Z_0$ 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 $\frac{\partial^n}{\partial x_{i_1} \ldots \partial x_{i_n}}$ 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

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

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

$$\partial_i\partial_j(fg) = (\partial_i\partial_j f)g + (\partial_i f)(\partial_j g) + (\partial_j f)(\partial_i g) + f(\partial_i\partial_j g).$$

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

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

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

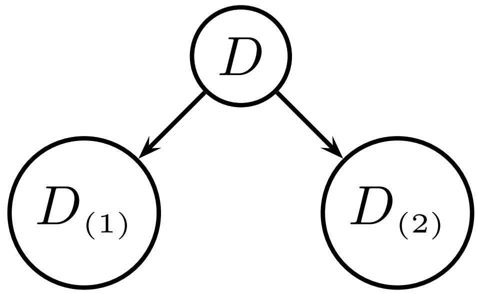
$$\Delta\partial_i\partial_j = \partial_i\partial_j \otimes \mathbf{1} + \partial_i \otimes \partial_j + \partial_j \otimes \partial_i + \mathbf{1} \otimes \partial_i\partial_j.$$

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

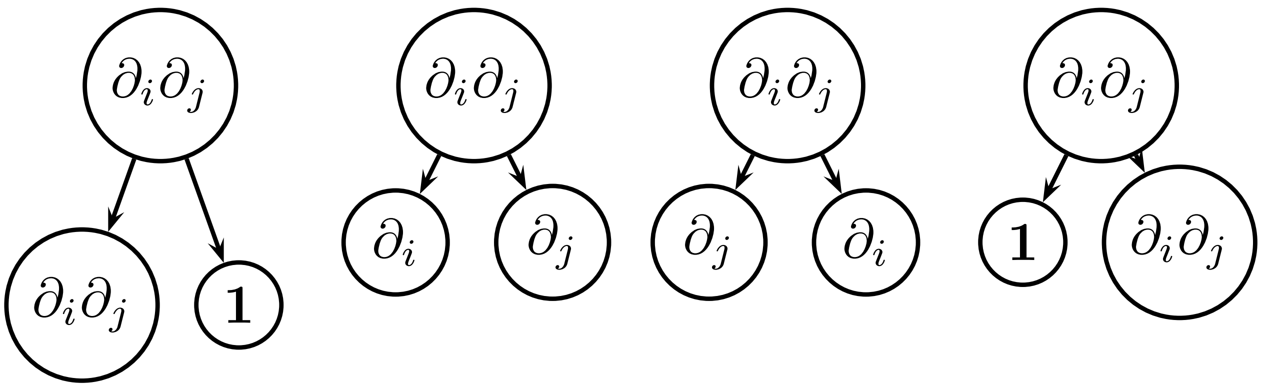
$$\Delta(\partial_i\partial_j) = (\partial_i \otimes \mathbf{1} + \mathbf{1} \otimes \partial_i)(\partial_j \otimes \mathbf{1} + \mathbf{1} \otimes \partial_j).$$

Coproduct: splitting into two parts

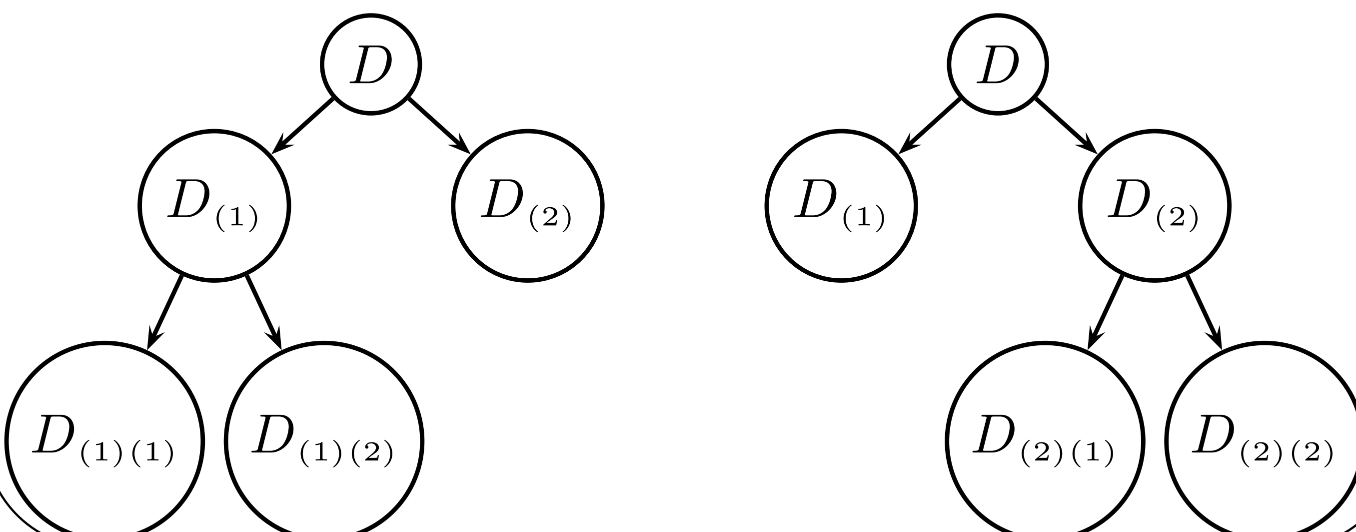
$$\Delta D = \sum D_{(1)} \otimes D_{(2)}$$



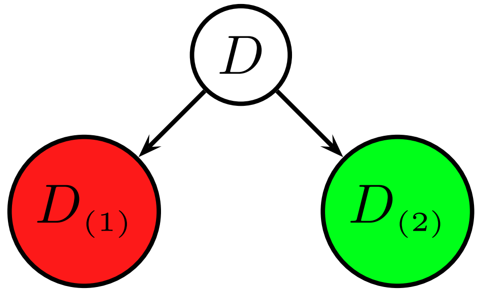
$$\Delta(\partial_i\partial_j) = \partial_i\partial_j \otimes \mathbf{1} + \partial_i \otimes \partial_j + \partial_j \otimes \partial_i + \mathbf{1} \otimes \partial_i\partial_j$$



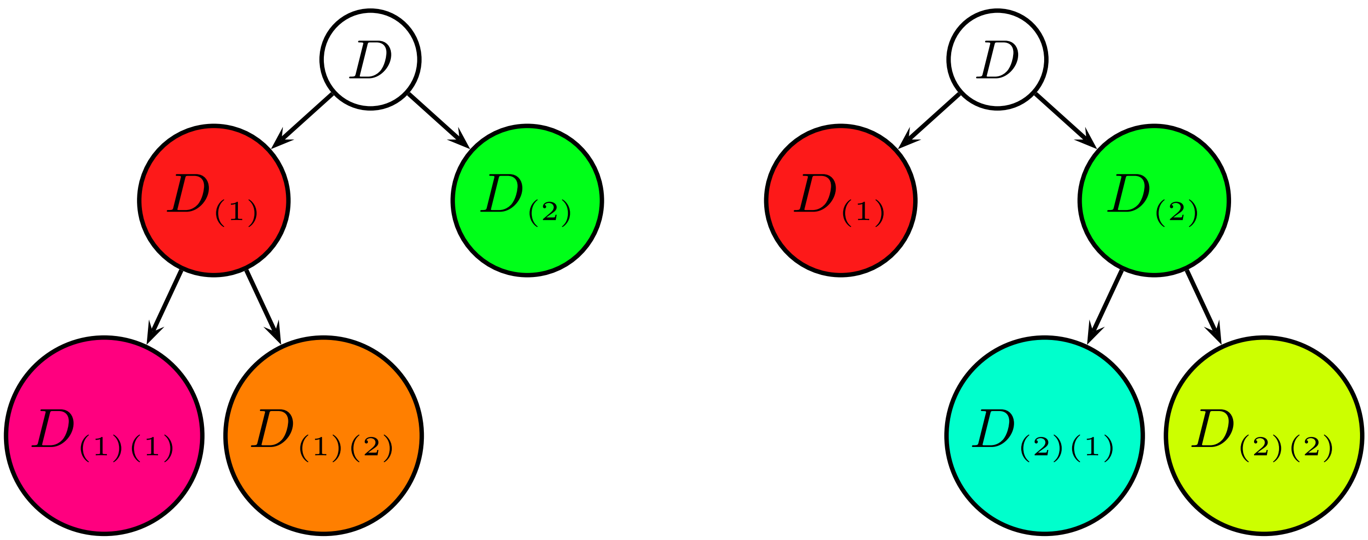
Splitting into three parts?



Coassociativity

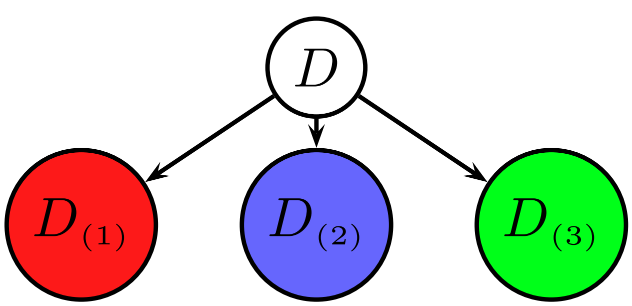


$$\Delta D = \sum D_{(1)} \otimes D_{(2)}$$



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

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



The Hopf algebra of derivations

Coassociativity

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

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

- $D(f_1 \ldots f_n) = \sum (D_{(1)} f_1) \ldots (D_{(n)} f_n)$.

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 $j(x)$

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

- Coproduct

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

- How to calculate Δe^{-iD} ?

Resummation of Δe^{-iD}

- Perturbative formula

$$\Delta e^{-iD} = 1\otimes 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \Delta D^n$$
$$= 1\otimes 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} D^n_{(1)} \otimes D^n_{(2)}$$

- Problem ΔD^n contains the term $1\otimes D^n$ so that Δe^{-iD} is an infinite series

- Reduced coproduct with respect to D:

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

- 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 $D^n_{(1')}$ and $D^n_{(2')}$ is at least n

Resummation of Δe^{-iD}

- Main identity

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

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

$$\Delta e^D = \sum_{n=0}^{\infty} \frac{1}{n!} D^n_{(1')} e^D \otimes D^n_{(2')} e^D$$
$$= (\Delta' e^D)(e^D \otimes e^D).$$

- Generating function

$$\frac{\delta Z}{\delta j(x)} = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \sum \Big(D^n_{(1')} e^{-iD} \frac{\delta W_0}{\delta j(x)} \Big) \Big(D^n_{(2')} e^{-iD} Z_0 \Big)$$
$$= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \sum \Big(D^n_{(1')} \frac{\delta W_1}{\delta j(x)} \Big) \Big(D^n_{(2')} Z \Big)$$

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

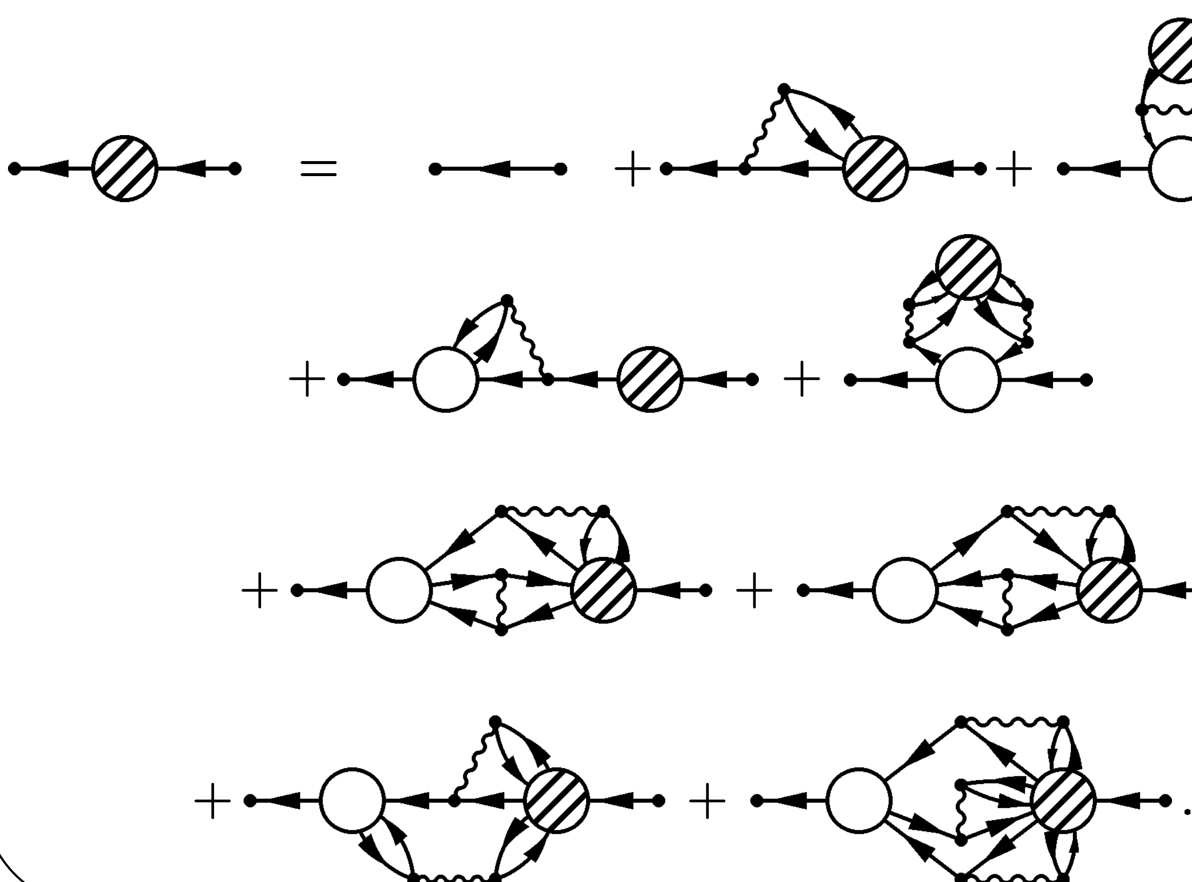
- The sum is now finite

Hierarchy of Green functions

- Green function

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

- 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

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

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

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

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

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

- In particular

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

Hierarchy of connected Green functions

- We define W by $Z = \mathrm{e}^W$
- We rewrite

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

- For connected Green functions

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

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

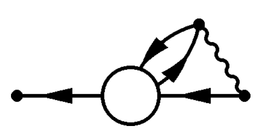
What is yet to be done

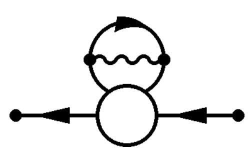
- Determine the structure of the Green functions
- Write Green functions in terms of one-particle irreducible vertices
- For the one-body Green function G
  - Closed shells $G = G^0 + G^0 \Sigma G$
  - Open shells (Hall 1974)

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

with

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

$\overleftarrow{\Sigma}$ =  $+ \ldots$

$\overleftrightarrow{\Sigma}$ =  $+ \ldots$

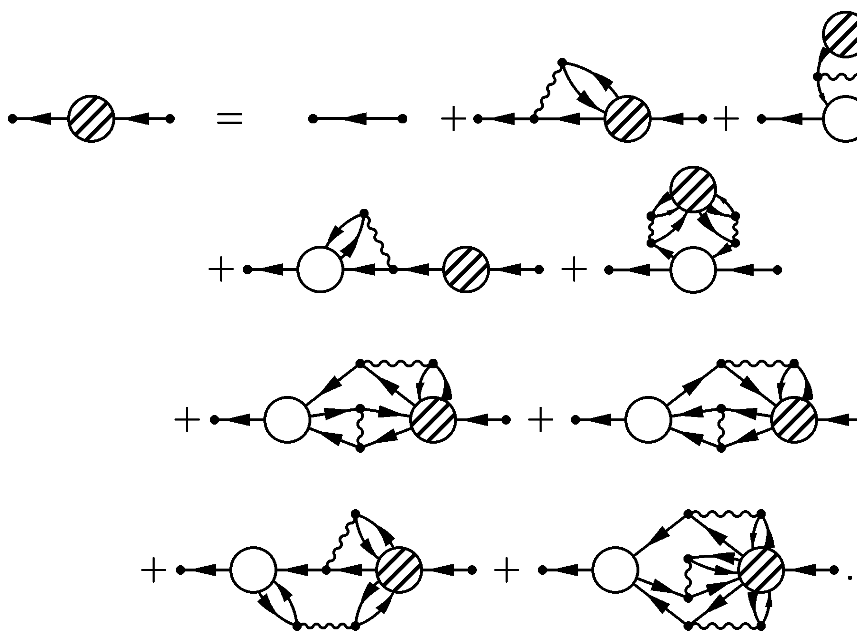
  - Closed shells: $\overleftarrow{\Sigma} = \overrightarrow{\Sigma} = \overleftrightarrow{\Sigma} = 0$

The self-energy: source of the problem

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

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

- 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

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

Signs of hope

- Define auxiliary Green functions

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

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

  with

$$\bar{G}^0 = \begin{pmatrix} G^0 & 1 \\ 1 & 0 \end{pmatrix},$$
$$\bar{G} = \begin{pmatrix} G & \overrightarrow{G} \\ \overleftarrow{G} & \overleftrightarrow{G} \end{pmatrix},$$
$$\bar{\Sigma} = \begin{pmatrix} \Sigma & \overrightarrow{\Sigma} \\ \overleftarrow{\Sigma} & \overleftrightarrow{\Sigma} \end{pmatrix}$$

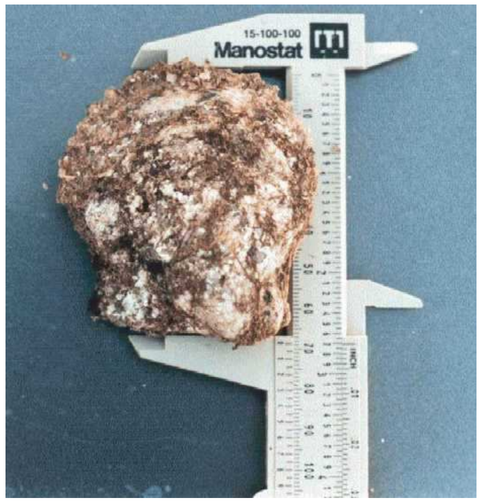
- $\bar{G}^0$ is now invertible

The Bethe-Salpeter equation

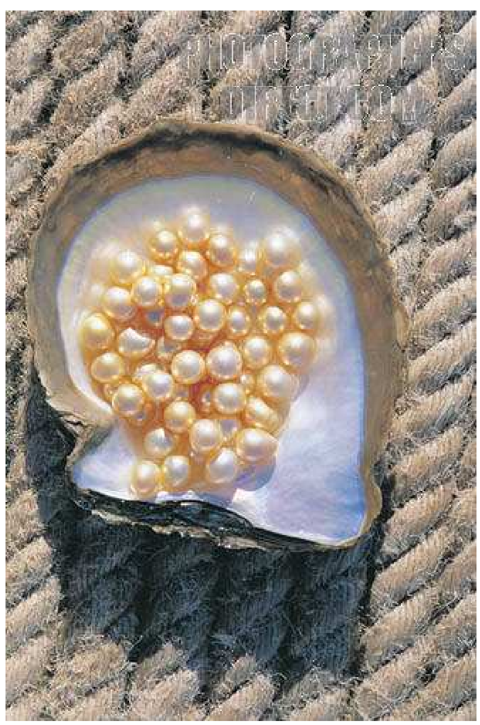
- Two-body Green function $G_2(x_1, x_2, y_1, y_2)$
- Closed shells $G_2 = G_1 G_1 + G_1 G_1 K G_2$
- K is a two-particle irreducible kernel
- Open shells ?
- Legendre transforms ?

Conclusion

- The closed-shell case is well mastered



- The open-shell case might reveal some pearls



The method of generating functions

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

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

- The S-matrix is

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

- Generating function

$$\begin{aligned} S(j) &= T\big({\rm e}^{-iA+i\int {\rm d}x\varphi(x)j(x)}\big) \\ &= \exp\Big(-iA(\frac{-i\delta}{\delta j(x)})\Big)T\big({\rm e}^{i\int {\rm d}x\varphi(x)j(x)}\big). \end{aligned}$$

The generating function for the Green functions

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

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

- Doubling of sources

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

- Generates the Green functions

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

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

$$Z(j) \quad = \quad \exp\Big(-iA(\frac{-i\delta}{\delta j_+(x)}) + iA(\frac{-i\delta}{\delta j_-(x)})\Big)$$
$$\mathrm{tr}\Big(\hat{\rho}\bar{T}\big(\mathrm{e}^{i\int \mathrm{d}x \varphi(x) j_-(x)}\big) T\big(\mathrm{e}^{i\int \mathrm{d}x \varphi(x) j_+(x)}\big)\Big)$$

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

- We want to calculate

$$
\begin{aligned}
Z(j) &= \exp\Big(-iA(\frac{-i\delta}{\delta j_+(x)}) + iA(\frac{-i\delta}{\delta j_-(x)})\Big) \\
&\quad \mathrm{tr}\Big(\hat{\rho}\bar{T}\big(\mathrm{e}^{i\int \mathrm{d}x\varphi(x)j_-(x)}\big)T\big(\mathrm{e}^{i\int \mathrm{d}x\varphi(x)j_+(x)}\big)\Big)
\end{aligned}
$$

- Compute the trace

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

with $K_\rho(j_+ + j_-) = \log\Big(\mathrm{tr}\big(\hat{\rho}{:}\mathrm{e}^{i\int \mathrm{d}x\varphi(x)(j_+(x)+j_-(x))}{:}\big)\Big)$

- Define the differential operator

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

- The generating function becomes

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