Properties of self energy and Luttinger-Ward functional

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Part I: Properties of Green's functions and the self-energy

Preliminaries

- We consider a a system of interacting Fermions with Hamiltonian

$$H = \sum_{\alpha,\beta} t_{\alpha,\beta}\, c_\alpha^\dagger c_\beta + \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha,\beta,\delta,\gamma}\, c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta.$$

- The indices α, $\beta \ldots$ are shorthand for some set of quantum numbers,

  in an LCAO description $\alpha = (\mathbf{k}, n, \sigma)$, with n orbital type such as Cu 3d$_{x^2-y^2}$, O 2p$_z$, Fe 3d$_{xy}$ ....
- We consider a grand canonical ensemble at inverse temperature $\beta = 1/k_B T$ and chemical potential μ
- Following Fetter-Walecka we define $K = H - \mu N \Rightarrow [K, N] = 0$
- The grand partition function is $Z =$ trace $\left(e^{-\beta K}\right)$
- Using the complete basis of eigenstates $K|i\rangle = K_i|i\rangle$, this becomes $Z = \sum_i e^{-\beta K_i}$
- The thermal average of an operator $\hat{O}$ is

$$\langle \hat{O} \rangle_{th} = \frac{1}{Z} \text{trace} \left(e^{-\beta K} \hat{O}\right) = \frac{1}{Z} \sum_i e^{-\beta K_i} \langle i|\hat{O}|i\rangle$$

Green's functions

Green's functions describe the following *gedanken experiment*

- Initially, the system is in thermal equilibrium
- 'Do something' to the system - i.e. act with some operator $\hat{B}$ - at time 0
- Let the system evolve under the action of H
- 'Undo the change' - i.e. act with some operator $\hat{A}$ - at some other time t
- Form the overlap with the undisturbed state at t

One can define different Green's functions but here we consider the retarded Green's function

$$G^R_{A,B}(t) \;=\; -i\Theta(t)\left(\langle\, \hat{A}(t)\hat{B}\,\rangle_{th} - (-1)^{n_B}\,\langle \hat{B}\hat{A}(t)\,\rangle_{th}\right)$$

Thereby

- $\hat{O}(t) = e^{itK/\hbar}\,\hat{O}\;e^{-itK/\hbar}$ (Heisenberg operator but with $H \rightarrow K = H - \mu N$)
- $n_B = [\hat{N}, \hat{B}]$ - the number of electrons added to the system by $\hat{B}$ - which may also be zero or negative

The retarded real-time Green's function has considerable physical significance

- Assume that the system is acted on by a small time dependent perturbation $H_1(t) = f(t)\hat{B}$
- Then the induced change in the expectation value of some operator $\hat{A}$ at time t is

$$\delta\langle\hat{A}\rangle(t) = \frac{1}{\hbar}\int_{-\infty}^{\infty} dt' \; G^R_{A,B}(t-t') \; f(t')$$

- $G^R_{A,B}(t)$ must be evaluated for the unperturbed system
- This is called linear-response theory or the Kubo formula
- The 'components' of $G^R_{A,B}$ such as $\langle \; \hat{A}(t)\hat{B} \; \rangle_{th}$ - so-called correlation functions - are 'related to' the spectra measured in inelastic scattering experiments
- For $\hat{B} = c_{\mathbf{k},\sigma}$ and $\hat{A} = c^{\dagger}_{\mathbf{k},\sigma}$ the Green's function is 'related to' the photoemission and inverse photoemission spectrum

Lehmann representation

We find (using $\sum_j |j\rangle\langle j| = 1$)

$$
\begin{aligned}
G^R_{A,B}(t) &= -i\Theta(t)\left(\langle\, \hat{A}(t)\hat{B}\,\rangle_{th} - (-1)^{n_B}\,\langle \hat{B}\hat{A}(t)\,\rangle_{th}\right)\\
&= -i\Theta(t)\,\frac{1}{Z}\left(\sum_i e^{-\beta K_i}\,\langle i|\,\hat{A}(t)\hat{B}\,|i\rangle - (-1)^{n_B}\,\sum_i e^{-\beta K_i}\,\langle i|\,\hat{B}\hat{A}(t)\,|i\rangle\right)\\
&= -i\Theta(t)\,\frac{1}{Z}\left(\sum_{i,j} e^{-\beta K_i}\,\langle i|\,\hat{A}(t)|j\rangle\langle j|\hat{B}\,|i\rangle - (-1)^{n_B}\,\sum_{i,j} e^{-\beta K_i}\,\langle i|\,\hat{B}|j\rangle\langle j|\hat{A}(t)\,|i\rangle\right)\\
&= -i\Theta(t)\,\frac{1}{Z}\left(\sum_{i,j} e^{-\beta K_i}\,\langle i|\,e^{\frac{it}{\hbar}K}\hat{A}e^{-\frac{it}{\hbar}K}|j\rangle\langle j|\hat{B}\,|i\rangle - (-1)^{n_B}\,\sum_{i,j} e^{-\beta K_i}\,\langle i|\,\hat{B}|j\rangle\langle j|e^{\frac{it}{\hbar}K}\hat{A}e^{-\frac{it}{\hbar}K}\,|i\rangle\right)\\
&= -i\Theta(t)\,\frac{1}{Z}\left(\sum_{i,j}\, e^{-\beta K_i}\;e^{\frac{it}{\hbar}(K_i-K_j)}\,\langle i|\hat{A}|j\rangle\;\langle j|\hat{B}|i\rangle - (-1)^{n_B}\,\sum_{i,j}\, e^{-\beta K_i}\;e^{\frac{it}{\hbar}(K_j-K_i)}\,\langle i|\hat{B}|j\rangle\;\langle j|\hat{A}|i\rangle\right)\\
&= -i\Theta(t)\,\frac{1}{Z}\sum_{i,j}\left(\, e^{-\beta K_i} - (-1)^{n_B}\,e^{-\beta K_j}\,\right)\,e^{\frac{it}{\hbar}(K_i-K_j)}\,\langle i|\hat{A}|j\rangle\;\langle j|\hat{B}|i\rangle
\end{aligned}
$$

The Fourier transform $G^R_{A,B}(\omega) \;=\; \int_{-\infty}^{\infty} e^{i\omega t}\,G^R_{A,B}(t)\,dt = \frac{1}{Z}\sum_{i,j}\frac{e^{-\beta K_i} - (-1)^{n_B}\,e^{-\beta K_j}}{\omega + i0^+ + \frac{1}{\hbar}(K_i - K_j)}\,\langle i|\hat{A}|j\rangle\;\langle j|\hat{B}|i\rangle$

The imaginary time Green's function

In the definition of the Heisenberg operator we replace $it \rightarrow \tau$: $\hat{O}(\tau) = e^{\tau K/\hbar}\, \hat{O}\, e^{-\tau K/\hbar}$

$$G_{A,B}(\tau) \;=\; -\langle\, T \left[\hat{A}(\tau)\; \hat{B} \right] \rangle_{th}$$

$$=\; -\; \Theta(\tau)\; \langle\; \hat{A}(\tau)\; \hat{B}\; \rangle_{th} - \Theta(-\tau)\; (-1)^{n_B}\; \langle\; \hat{B}\; \hat{A}(\tau)\; \rangle_{th}$$

We recall ....

$$G^R_{A,B}(t) \;=\; -i\; \Theta(t)\; \langle\; \hat{A}(t)\; \hat{B}\; \rangle_{th} -\; i\; \Theta(t)\; (-1)^{n_B}\; \langle \hat{B}\; \hat{A}(t)\; \rangle_{th}$$

.... and by similar manipulations as in the preceding slide we find the Lehmann representation

$$G_{A,B}(\tau) \;=\; -\,\frac{1}{Z} \sum_{i,j} \big(\; \Theta(\tau)\; e^{-\beta K_i} - (-1)^{n_B}\; \Theta(-\tau) e^{-\beta K_j}\; \big)\;\; e^{\frac{\tau}{\hbar}(K_i - K_j)}\; \langle i|\hat{A}|j\rangle\; \langle j|\hat{B}|i\rangle$$

Domain of existence

We had

$$G_{A,B}(\tau) \;=\; -\frac{1}{Z}\sum_{i,j}\;\Big(\,\Theta(\tau)\,e^{-\beta K_i} - (-1)^{n_B}\,\Theta(-\tau)e^{-\beta K_j}\,\Big)\;e^{\frac{\tau}{\hbar}(K_i-K_j)}\;\langle i|\hat{A}|j\rangle\;\langle j|\hat{B}|i\rangle$$

τ-dependence, $\tau > 0$: $e^{-\beta K_i}\; e^{\frac{\tau}{\hbar}(K_i-K_j)} = e^{-\beta K_i}\; e^{\frac{|\tau|}{\hbar}(K_i-K_j)} = e^{(\frac{|\tau|}{\hbar}-\beta)K_i}\; e^{-\frac{|\tau|}{\hbar}K_j}$

τ-dependence, $\tau < 0$: $e^{-\beta K_j}\; e^{\frac{\tau}{\hbar}(K_i-K_j)} = e^{-\beta K_j}\; e^{\frac{|\tau|}{\hbar}(K_j-K_i)} = e^{(\frac{|\tau|}{\hbar}-\beta)K_j}\; e^{-\frac{|\tau|}{\hbar}K_i}$

K_i, K_j are eigenvalues of $H - \mu N$ - in the thermodynamical limit they are bounded from below - namely by K_0 - but unbounded from above

$\Rightarrow G_{A,B}(\tau)$ is well defined only for $-\hbar\beta < \tau < \hbar\beta$

Fourier transform

- $G_{A,B}(\tau)$ exists only in the intervall $[-\hbar\beta : \hbar\beta]$

  $\Rightarrow$ it can be expanded in a Fourier series with frequencies $\omega_\nu = \nu \dfrac{2\pi}{2\hbar\beta} = \dfrac{\nu\pi}{\hbar\beta}$

$$G_{A,B}(\tau) \;=\; \frac{1}{\hbar\beta} \sum_{\nu=-\infty}^{\infty} e^{-i\omega_\nu \tau}\, G_{A,B}(i\omega_\nu),$$

$$G_{A,B}(i\omega_\nu) \;=\; \int_0^{\hbar\beta} d\tau\; e^{i\omega_\nu \tau}\, G_{A,B}(\tau),$$

- One can show that for $\tau \in [-\hbar\beta, 0]$ one has $G_{A,B}(\tau + \hbar\beta) = (-1)^{n_B}\, G_{A,B}(\tau)$

  $\Rightarrow e^{-i\omega_\nu \cdot \hbar\beta} = e^{-i\nu\pi} = (-1)^{n_B} \Rightarrow$ only even ν for even n_B, only odd ν for odd n_B

- The ω_ν are called Matsubara frequencies

- By straightforward calculation we find the Fourier transform

$$G_{A,B}(i\omega_\nu) \;=\; \int_0^{\hbar\beta} d\tau\; e^{i\omega_\nu \tau}\, G_{A,B}(\tau) = \frac{1}{Z} \sum_{i,j} \frac{e^{-\beta K_i} - (-1)^{n_B}\, e^{-\beta K_j}}{i\omega_\nu + \frac{1}{\hbar}(K_i - K_j)} \,\langle i|\hat{A}|j\rangle\, \langle j|\hat{B}|i\rangle$$

'The' Green's function

We found

$$G_{A,B}(i\omega_\nu) \;=\; \frac{1}{Z}\sum_{i,j} \frac{e^{-\beta K_i} - (-1)^{n_B}\, e^{-\beta K_j}}{i\omega_\nu + \frac{1}{\hbar}(K_i - K_j)}\, \langle i|\hat{A}|j\rangle\, \langle j|\hat{B}|i\rangle.$$

Now recall the Fourier transform of the retarded real-time Green's function

$$G^R_{A,B}(\omega) \;=\; \frac{1}{Z}\sum_{i,j} \frac{e^{-\beta K_i} - (-1)^{n_B}\, e^{-\beta K_j}}{\omega + i0^+ + \frac{1}{\hbar}(K_i - K_j)}\, \langle i|\hat{A}|j\rangle\, \langle j|\hat{B}|i\rangle$$

$G^R_{A,B}(\omega)$ can be obtained from $G_{A,B}(i\omega_\nu)$ by replacing $i\omega_\nu \rightarrow \omega + i0^+$

This means that there is one function $G_{AB}(z)$ of the complex frequency z which gives the imaginary-time Green's function when evaluated at the Matsubara frequencies, $z = i\omega_\nu$, and the retarded real-time Green's function when evaluated along a line infinitesimally above the real axis, $z = \omega + i0^+$

This function which is defined in the whole complex frequency plane is often called 'the' Green's function

Importance of the imaginary-time Green's function

The relation between the Fourier transforms of the time-ordered imaginary-time Green's function and the real-time retarded Green's function is the main reason why imaginary-time Green's functions are considered in the first place

The time-ordered imaginary-time Green's function can be expanded into Feynman-diagrams whereas this is not possible for real-time Green's functions at finite temperature

A standard procedure - used frequently in the literature - therefore is to evaluate the imaginary Green's function, often using e.g. a partial summation of Feynman diagrams. This gives some function $G_{approx}(i\omega_\nu)$ in which one replaces $i\omega_\nu \rightarrow \omega + i0^+$ ('analytical continuation') to obtain the real-time Green's function

The question of whether the full Green's function is uniquely defined by its values at the Matsubara frequencies has been answered affirmatively by G. Baym and N. D. Mermin, J. Math. Phys. **2**,232 (1961)

The single-particle Green's function

We recall the definition of 'the' Green's function

$$G_{A,B}(z) \;=\; \frac{1}{Z}\sum_{i,j}\; e^{-\beta K_i}\;\left[\;\frac{\langle i|\hat{A}|j\rangle\;\langle j|\hat{B}|i\rangle}{z+\frac{1}{\hbar}(K_i-K_j)} - (-1)^{n_B}\frac{\langle i|\hat{B}|j\rangle\langle j|\hat{A}|i\rangle}{z+\frac{1}{\hbar}(K_j-K_i)}\;\right]$$

We specialize to the single-particle Green's function which corresponds to $\hat{A}=c_\alpha$, $\hat{B}=c_\beta^\dagger$ so that $n_B=1$

$$G_{\alpha,\beta}(z) \;=\; \frac{1}{Z}\sum_{i,j}\; e^{-\beta K_i}\left[\;\frac{\langle i|c_\alpha|j\rangle\langle j|c_\beta^\dagger|i\rangle}{z-\frac{1}{\hbar}(K_j-K_i)}+\frac{\langle i|c_\beta^\dagger|j\rangle\langle j|c_\alpha|i\rangle}{z-\frac{1}{\hbar}(K_i-K_j)}\;\right]$$

We recall that $\alpha=(\mathbf{k},n,\sigma)$ - $G_{\alpha,\beta}(z)$ may be viewed as a matrix of dimension $n_{orb}\times n_{orb}$ where n_{orb} is the number of α in the system - we will often write this as $\mathbf{G}(z)$

The 1^{st} term describes adding an electron and removing it - inverse photoemission

The 2^{nd} term describes removing an electron and adding it - photoemission

Spectral densities

$$G_{\alpha,\beta}(z) \;=\; \frac{1}{Z}\sum_{i,j} e^{-\beta K_i}\left[\frac{\langle i|c_\alpha|j\rangle\langle j|c_\beta^\dagger|i\rangle}{z-\frac{1}{\hbar}(K_j-K_i)}+\frac{\langle i|c_\beta^\dagger|j\rangle\langle j|c_\alpha|i\rangle}{z-\frac{1}{\hbar}(K_i-K_j)}\right]=\int_{-\infty}^{\infty}d\omega\;\frac{\rho^{(+)}_{\alpha,\beta}(\omega)}{z-\omega}+\int_{-\infty}^{\infty}d\omega\;\frac{\rho^{(-)}_{\alpha,\beta}(\omega)}{z-\omega}$$

whereby

$$\rho^{(+)}_{\alpha,\beta}(\omega) \;=\; \frac{1}{Z}\sum_{i,j} e^{-\beta K_i}\;\langle i|c_\alpha|j\rangle\langle j|c_\beta^\dagger|i\rangle\;\delta\left(\omega-\frac{1}{\hbar}(K_j-K_i)\right)$$

$$\rho^{(-)}_{\alpha,\beta}(\omega) \;=\; \frac{1}{Z}\sum_{i,j} e^{-\beta K_i}\;\langle i|c_\beta^\dagger|j\rangle\langle j|c_\alpha|i\rangle\;\delta\left(\omega-\frac{1}{\hbar}(K_i-K_j)\right)$$

Then

$$\int_{-\infty}^{\infty}d\omega\;\rho^{(-)}_{\alpha,\beta}(\omega) \;=\; \frac{1}{Z}\sum_{i,j} e^{-\beta K_i}\;\langle i|c_\beta^\dagger|j\rangle\langle j|c_\alpha|i\rangle=\frac{1}{Z}\sum_{i} e^{-\beta K_i}\;\langle i|c_\beta^\dagger c_\alpha|i\rangle=\langle c_\beta^\dagger c_\alpha\rangle_{th}$$

Dito:

$$\int_{-\infty}^{\infty}d\omega\;\rho^{(+)}_{\alpha,\beta}(\omega) \;=\; \langle c_\alpha c_\beta^\dagger\rangle_{th}$$

If we define $\rho=\rho^{(+)}+\rho^{(-)}$

$$\int_{-\infty}^{\infty}d\omega\;\rho_{\alpha,\beta}(\omega) \;=\; \langle\left\{c_\alpha,c_\beta^\dagger\right\}\rangle_{th}=\delta_{\alpha,\beta}$$

We recall

$$\rho^{(+)}_{\alpha,\beta}(\omega) \;=\; \frac{1}{Z}\sum_{i,j}\; e^{-\beta K_i}\;\langle i|c_\alpha|j\rangle\langle j|c^\dagger_\beta|i\rangle\;\delta\left(\omega-\frac{1}{\hbar}(K_j-K_i)\right)$$

$$\rho^{(-)}_{\alpha,\beta}(\omega) \;=\; \frac{1}{Z}\sum_{i,j}\; e^{-\beta K_i}\;\langle i|c^\dagger_\beta|j\rangle\langle j|c_\alpha|i\rangle\;\delta\left(\omega-\frac{1}{\hbar}(K_i-K_j)\right)$$

- The labels i and j denote eigenstates of the Hamiltonian
- For a finite system the eigenenergies are discrete and the $\rho(\omega)$ are 'sums of δ-spikes'
- In the thermodynamical limit the spacing between eigenenergies rapidly approaches zero and i and j become co
- At the same time the matrix elements $\langle i|c_\alpha|j\rangle$ vanish and the sums over i and j become integrals

Then e.g.

$$\begin{aligned}\rho^{(+)}_{\alpha,\beta}(\omega) \;&=\; \frac{1}{Z}\int dK_1\;\int dK_2\; e^{-\beta K_1}\;F(K_1,K_2)\;\delta\left(\omega-\frac{1}{\hbar}(K_1-K_2)\right)\\ &=\; \frac{\hbar}{Z}\int dK_1\;\; e^{-\beta K_1}\;F(K_1,K_1-\hbar\omega)\end{aligned}$$

The $\rho(\omega)$ become continuous functions

Asymptotic behavior

We recall....

$$G_{\alpha,\beta}(z) = \frac{1}{Z}\sum_{i,j} e^{-\beta K_i}\left[\frac{\langle i|c_\alpha|j\rangle\langle j|c_\beta^\dagger|i\rangle}{z+\frac{1}{\hbar}(K_i-K_j)} + \frac{\langle i|c_\beta^\dagger|j\rangle\langle j|c_\alpha|i\rangle}{z+\frac{1}{\hbar}(K_j-K_i)}\right]$$

.... and consider the limit $|z|\rightarrow\infty$ - then

$$\frac{1}{z+\frac{1}{\hbar}(K_j-K_i)} \rightarrow \frac{1}{z} - \frac{K_j-K_i}{\hbar z^2} + O\left(\frac{1}{z^3}\right).$$

The first term gives

$$\frac{1}{zZ}\sum_i e^{-\beta K_i}\left[\langle i|c_\alpha c_\beta^\dagger|i\rangle + \langle i|c_\beta^\dagger c_\alpha|i\rangle\right] = \frac{1}{z}\langle\{c_\beta^\dagger, c_\alpha\}\rangle_{th} = \frac{\delta_{\alpha,\beta}}{z}$$

The second term gives

$$-\frac{1}{\hbar z^2 Z}\sum_{i,j} e^{-\beta K_i}\left[(K_i-K_j)\langle i|c_\alpha|j\rangle\langle j|c_\beta^\dagger|i\rangle + (K_j-K_i)\langle i|c_\beta^\dagger|j\rangle\langle j|c_\alpha|i\rangle\right]$$

Now we use $(K_j-K_i)\langle j|c_\alpha|i\rangle = \langle j|Kc_\alpha - c_\alpha K|i\rangle = \langle j|\;[K,c_\alpha]\;|i\rangle$ and find

$$-\frac{1}{\hbar z^2 Z}\sum_i e^{-\beta K_i}\left[\langle i|\;[K,c_\alpha]\;c_\beta^\dagger\;|i\rangle + \langle i|\;c_\beta^\dagger\;[K,c_\alpha]\;|i\rangle\right] = \frac{\left\langle\left\{c_\beta^\dagger,[c_\alpha,K]\right\}\right\rangle_{th}}{\hbar z^2}$$

For our Hamiltonian

$$K = \sum_{\alpha,\beta} t_{\alpha,\beta}\, c_\alpha^\dagger c_\beta - \mu \sum_\alpha\, c_\alpha^\dagger c_\alpha + \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha,\beta,\delta,\gamma}\, c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$$

we find

$$\left\langle \left\{ c_\beta^\dagger, [c_\alpha, K] \right\} \right\rangle_{th} = t_{\alpha,\beta} - \mu\, \delta_{\alpha,\beta} + \sum_{\gamma,\delta} \left(V_{\alpha,\gamma,\beta,\delta} - V_{\alpha,\gamma,\delta,\beta}\right) \left\langle c_\gamma^\dagger c_\delta \right\rangle_{th}$$

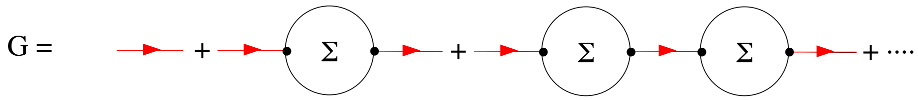
$$= t_{\alpha,\beta} - \mu\, \delta_{\alpha,\beta} + V_{\alpha,\beta}^{(HF)}$$

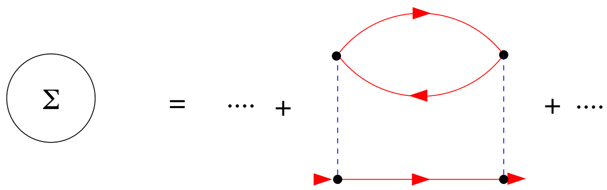
All in all we find the asymptotic expression for $|z| \to \infty$

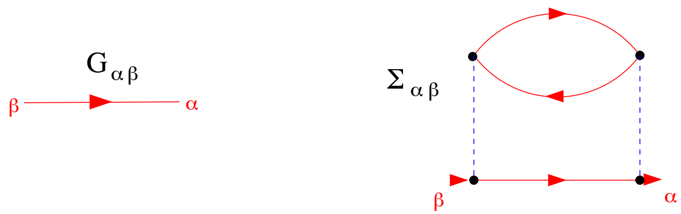
$$\mathbf{G}(z) \to \frac{1}{z} + \frac{\mathbf{t} - \mu + \mathbf{V}^{(HF)}}{\hbar z^2} + O\left(\frac{1}{z^3}\right).$$

The self-energy

The time-ordered imaginary-time Green's functions can be expanded in Feynman diagrams - this allows to introduce the self-energy ....







.... and we can read off the Dyson equation (note that we already replaced $i\omega_\nu \to z$ throughout)

$$\mathbf{G}^{-1}(z) \;=\; \mathbf{G}_0^{-1}(z) - \mathbf{\Sigma}(z) = z - \frac{\mathbf{t} - \mu}{\hbar} - \mathbf{\Sigma}(z)$$

($\mathbf{t}$ is the matrix $t_{\alpha,\beta}$ in $H = \sum_{\alpha,\beta} \; t_{\alpha,\beta} \; c_\alpha^\dagger c_\beta + \ldots$)

The Dyson equation was

$$\mathbf{G}^{-1}(z) \;=\; z - \frac{\mathbf{t}-\mu}{\hbar} - \mathbf{\Sigma}(z)$$

Now we recall the asymptotic expression

$$\mathbf{G}(z) \to \frac{1}{z} + \frac{\mathbf{t}-\mu+\mathbf{V}^{(HF)}}{\hbar z^2} + O\left(\frac{1}{z^3}\right) \;\Rightarrow\; \mathbf{G}^{-1}(z) \to z - \frac{\mathbf{t}-\mu}{\hbar} - \frac{\mathbf{V}^{(HF)}}{\hbar} + O\left(\frac{1}{z}\right)$$

It follows that

$$\mathbf{\Sigma}(z) \to \frac{\mathbf{V}^{(HF)}}{\hbar} + O\left(\frac{1}{z}\right)$$

If we define

$$\mathbf{\Sigma}(z) = \frac{\mathbf{V}^{(HF)}}{\hbar} + \mathbf{\Sigma}_{res}(z) \;\Rightarrow\; \mathbf{\Sigma}_{res}(z) \to \frac{1}{z}$$

In particular for Hubbard-type models $\mathbf{V}^{(HF)} = U n_{\bar{\sigma}}$

Analytical properties

The single particle Green's function $\mathbf{G}(z)$ - and hence also the self-energy $\mathbf{\Sigma}(z)$ are defined in the whole complex z-plane - we now want to discuss general properties of these functions

For simplicity we restrict ourselves to the single-band case that means $\alpha = (\mathbf{k}, \sigma)$ -if wave vector and z-spin are conserved we have $G_{\alpha,\beta} \propto \delta_{\alpha,\beta}$ so that

$$G_\alpha(z) \;=\; \int_{-\infty}^{\infty} d\omega\; \frac{\rho_\alpha^{(+)}(\omega)}{z-\omega} + \int_{-\infty}^{\infty} d\omega\; \frac{\rho_\alpha^{(-)}(\omega)}{z-\omega}$$

$$\rho_\alpha^{(+)}(\omega) \;=\; \frac{1}{Z}\sum_{i,j} e^{-\beta K_i} \quad |\langle j|c_\alpha^\dagger|i\rangle|^2 \quad \delta\left(\omega - \frac{1}{\hbar}(K_j - K_i)\right)$$

$$\rho_\alpha^{(-)}(\omega) \;=\; \frac{1}{Z}\sum_{i,j} e^{-\beta K_i} \quad |\langle j|c_\alpha|i\rangle|^2 \quad \delta\left(\omega - \frac{1}{\hbar}(K_i - K_j)\right)$$

The functions $\rho_\alpha^{(+)}(\omega)$ and $\rho_\alpha^{(-)}(\omega)$ are real and positive $\Rightarrow (G_\alpha(z))^* = G_\alpha(z^*)$

We had (with $\rho_\alpha(\omega) = \rho^{(+)}(\omega) + \rho^{(-)}(\omega)$, real and positive and $\int d\omega\ \rho_\alpha(\omega) = 1$):

$$G_\alpha(z) \;=\; \int_{-\infty}^{\infty} d\omega\ \frac{\rho_\alpha(\omega)}{z-\omega}$$

Put $z = x + iy$ - the imaginary part of $G_\alpha(z)$ is

$$\mathcal{I}G_\alpha(x+iy) \;=\; -\int_{-\infty}^{\infty} d\omega\ \frac{y\rho_\alpha(\omega)}{(x-\omega)^2+y^2} \qquad \begin{cases} <0 & y>0 \\ >0 & y<0 \end{cases}$$

$G_\alpha(z)$ has no zeros off the real axis $\Rightarrow$ $G_\alpha^{-1}(z)$ is regular (has no poles) off the real axis

From the Dyson equation ....

$$G_\alpha^{-1}(z) \;=\; z - \frac{t_\alpha - \mu}{\hbar} - \frac{V^{(HF)}}{\hbar} - \Sigma_{res}(z)$$

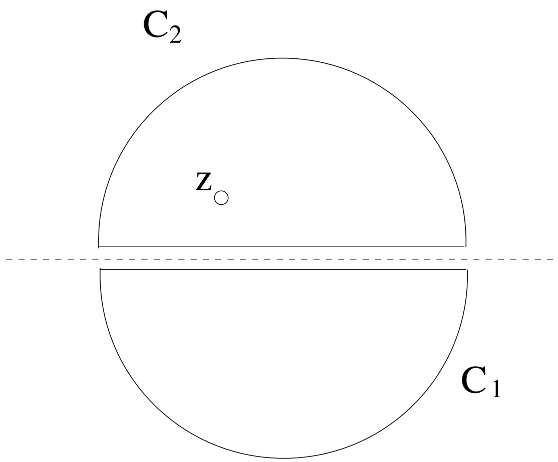
.... it follows that $\Sigma_{res}(z)$ is regular off the real axis

Moreover we had $(G_\alpha(z))^* = G_\alpha(z^*) \Rightarrow \left(G_\alpha^{-1}(z)\right)^* = G_\alpha^{-1}(z^*)$

$$z^* - \frac{t_\alpha - \mu}{\hbar} - \frac{V^{(HF)}}{\hbar} - (\mathbf{\Sigma}_{res}(z))^* \;=\; z^* - \frac{t_\alpha - \mu}{\hbar} - \frac{V^{(HF)}}{\hbar} - \mathbf{\Sigma}_{res}(z^*)$$

$$\Rightarrow (\mathbf{\Sigma}_{res}(z))^* = \mathbf{\Sigma}_{res}(z^*)$$

In summary:



- $\Sigma(z) = \frac{V^{(HF)}}{\hbar} + \Sigma_{res}(z)$
- $\Sigma_{res}(z) \to \frac{C}{z}$
- $\Sigma_{res}(z)$ is analytical off the real axis
- $(\Sigma_{res}(z))^* = \Sigma_{res}(z^*)$

Now define for real ω (with real $K(\omega)$ and $J(\omega)$)

$$\lim_{\epsilon\to 0^+} \Sigma_{res}(\omega + i\epsilon) = K(\omega) - iJ(\omega) \;\Rightarrow\; \lim_{\epsilon\to 0^+} \Sigma_{res}(\omega - i\epsilon) = K(\omega) + iJ(\omega)$$

For z in the upper plane

$$\oint_{C_1} dz' \, \frac{\Sigma_{res}(z')}{z' - z} = 0 \;\Rightarrow\; \int_{-\infty}^{\infty} d\omega \, \frac{K(\omega) + iJ(\omega)}{\omega - z} = 0 \Rightarrow \int_{-\infty}^{\infty} d\omega \, \frac{K(\omega)}{\omega - z} = -\int_{-\infty}^{\infty} d\omega \, \frac{iJ(\omega)}{\omega - z}$$

Now use Cauchy's theorem

$$\Sigma_{res}(z) = \frac{1}{2\pi i} \oint_{C_2} dz' \, \frac{\Sigma_{res}(z')}{z' - z} = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega \, \frac{K(\omega) - iJ(\omega)}{\omega - z} \;\Rightarrow\; \Sigma_{res}(z) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \, \frac{J(\omega)}{z - \omega}$$

We thus arrive at the spectral representation of the full self-energy

(J.M. Luttinger, Phys. Rev. **121**, 942 (1961)):

$$\Sigma(z) \;=\; \frac{V^{(HF)}}{\hbar} + \int_{-\infty}^{\infty} d\omega \, \frac{\sigma(\omega)}{z-\omega}$$

(with $\sigma(\omega) = \frac{1}{\pi} J(\omega)$, real and positive)

Summary, spectral representation

Green's function

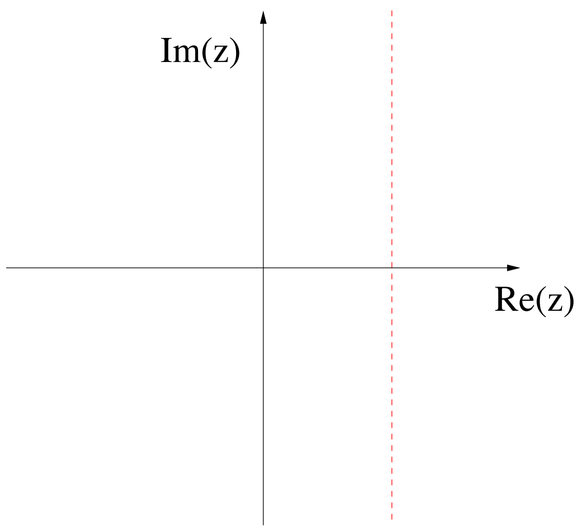
$$G_\alpha(z) = \int_{-\infty}^{\infty} d\omega \, \frac{\rho_\alpha(\omega)}{z-\omega}$$

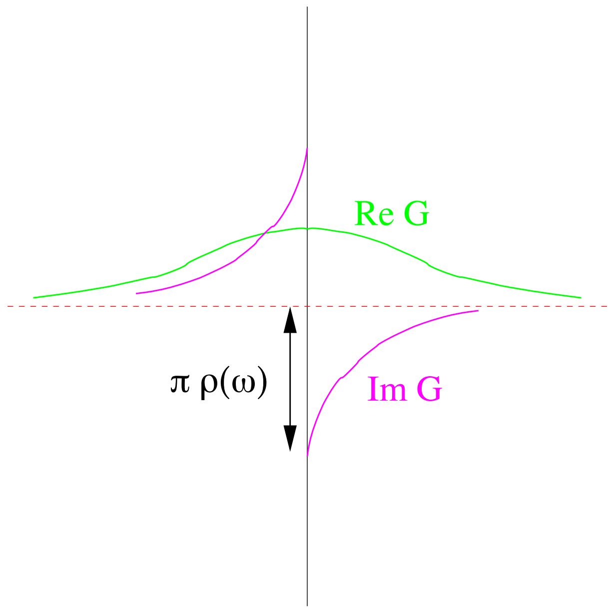
- $\rho_\alpha(\omega)$ is real and positive
- $G_\alpha(z) \to \frac{1}{z}$
- Analytical off the real axis

Self energy

$$\Sigma_\alpha(z) = \frac{V^{(HF)}}{\hbar} + \int_{-\infty}^{\infty} d\omega \, \frac{\sigma_\alpha(\omega)}{z-\omega}$$

- $\sigma_\alpha(\omega)$ is real and positive
- $\Sigma_\alpha(z) \to \frac{V^{(HF)}}{\hbar} + \frac{C}{z}$
- Analytical off the real axis





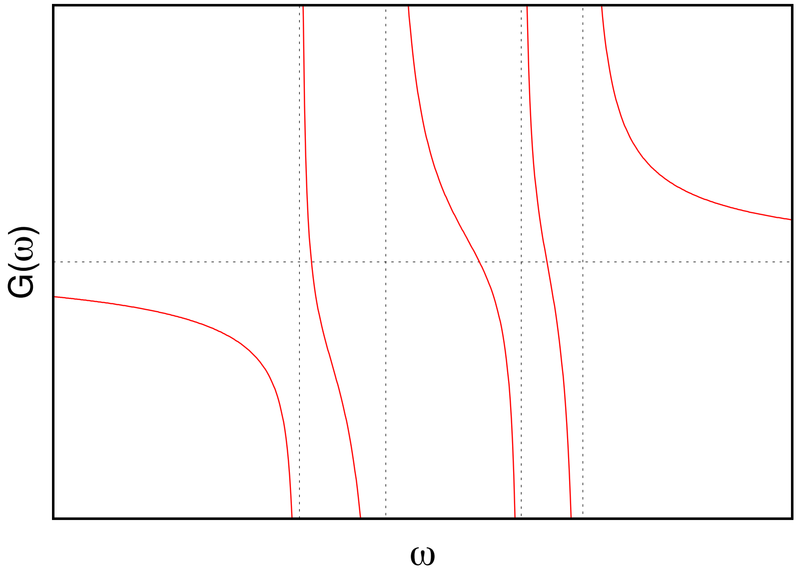
For a finite system we expect the self-energy also to be discrete

$$\Sigma_\alpha(z) = \frac{V_\alpha^{(HF)}}{\hbar} + \sum_{i=1}^{m} \frac{\sigma_i}{z - \zeta_i}$$

The Greens function therefore is

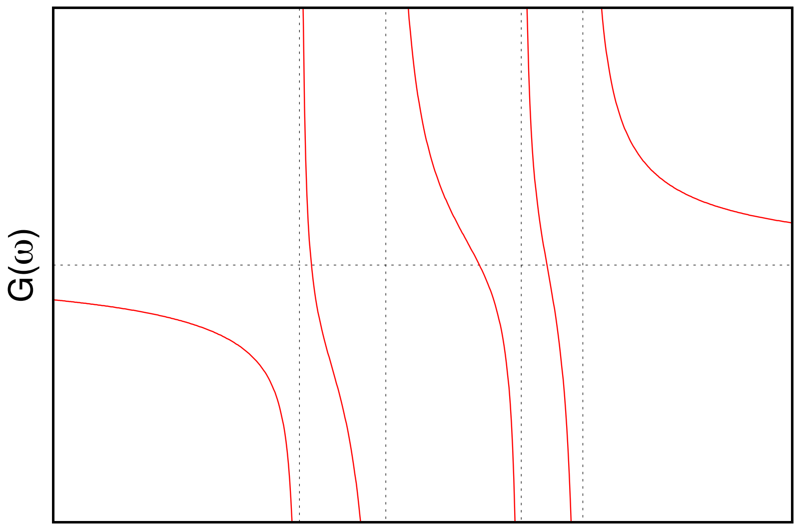
$$G(\omega) = \left(\omega - \frac{t_\alpha - \mu + V_\alpha^{(HF)}}{\hbar} - \sum_{i=1}^{m} \frac{\sigma_i}{z - \zeta_i} \right)^{-1} = \left(\omega - \epsilon_\alpha - \sum_{i=1}^{m} \frac{\sigma_i}{z - \zeta_i} \right)^{-1}$$

Now consider again the Green's function:



The ζ_i are the zeros of $G(\omega)$

It follows that the poles of $\Sigma(\omega)$ are 'sandwiched' in between the poles of $G(\omega)$ - $m = n - 1$



Near a zero ζ_i : $G(\omega) = a_i(\omega - \zeta_i) + b_i(\omega - \zeta_i)^2 + \ldots$ and

$$\begin{aligned} G^{-1}(\omega) &= \omega - \epsilon_\alpha - \sum_j \frac{\sigma_j}{z - \zeta_j} \\ &= -\frac{\sigma_i}{\omega - \zeta_i} + \omega - \epsilon_\alpha - \sum_{j \neq i} \frac{\sigma_j}{z - \zeta_j} \\ &= -\frac{\sigma_i}{\omega - \zeta_i} + c_0 + c_1(\omega - \zeta_i) + \ldots \end{aligned}$$

with real constants c_0 and c_1 - therefore

$$G(\omega) = -\frac{\omega - \zeta_i}{\sigma_i} - \frac{c_0}{\sigma_i^2}(\omega - \zeta_i)^2 + \ldots, \Rightarrow a_i = -\frac{1}{\sigma_i}.$$

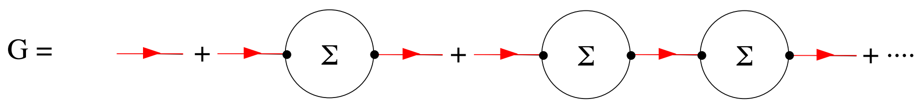
Part II: The Luttinger-Ward functional

Our Hamiltonian from now on

$$H_0 = \sum_{\mathbf{k}} \sum_{\alpha,\beta} \mathbf{t}_{\alpha,\beta}(\mathbf{k})\, c^\dagger_{\mathbf{k},\alpha}\, c_{\mathbf{k},\beta}$$

$$H_1 = \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q})\, c^\dagger_{\mathbf{k}+\mathbf{q},\alpha}\, c^\dagger_{\mathbf{k}'-\mathbf{q},\beta}\, c_{\mathbf{k}',\gamma}\, c_{\mathbf{k},\delta}$$

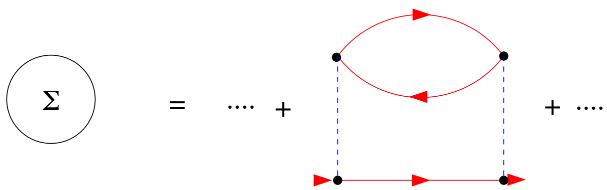
- α, β etc label the atom and orbital in the unit cell (e.g. Cu 3d$_{x^2-y^2}$, O 2p$_z$, Fe 3d$_{xy}$) and the spin
- The number of such orbitals per unit-cell is n_{orb}
- The eigenvalues $E_n(\mathbf{k})$ of $\mathbf{t}(\mathbf{k})$ give the noninteracting band structure

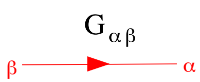


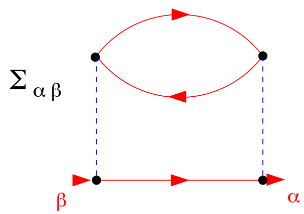
In $G_{\alpha,\beta}$, $\Sigma_{\alpha,\beta}$

α outgoing

β incoming







The Grand Canonical Potential

The Grand Canonical Potential $\Omega = U - TS - \mu N$ is obtained from the Grand Partition Function Z

$$\Omega \;=\; -\frac{1}{\beta}\, log(Z)$$

It gives the thermodynamics of the system: $S = -\left(\frac{\partial\Omega}{\partial T}\right)_{V,\mu}$, $p = -\left(\frac{\partial\Omega}{\partial V}\right)_{T,\mu}$, $N = -\left(\frac{\partial\Omega}{\partial \mu}\right)_{T,V}$

Ω can be evaluated analytically for some systems e.g. for noninteracting Bloch electrons:

$$\Omega \;=\; -\frac{1}{\beta}\;\sum_{n=1}^{2n_{orb}}\sum_{\mathbf{k}} \ln\left(1 + e^{-\beta(E_n(\mathbf{k})-\mu)}\right)$$

- n_{orb} number of orbitals per unit cell, $2n_{orb}$ the number of bands
- $E_n(\mathbf{k})$: Dispersion of n^{th} band
- Gives for example: $C_v \propto T$

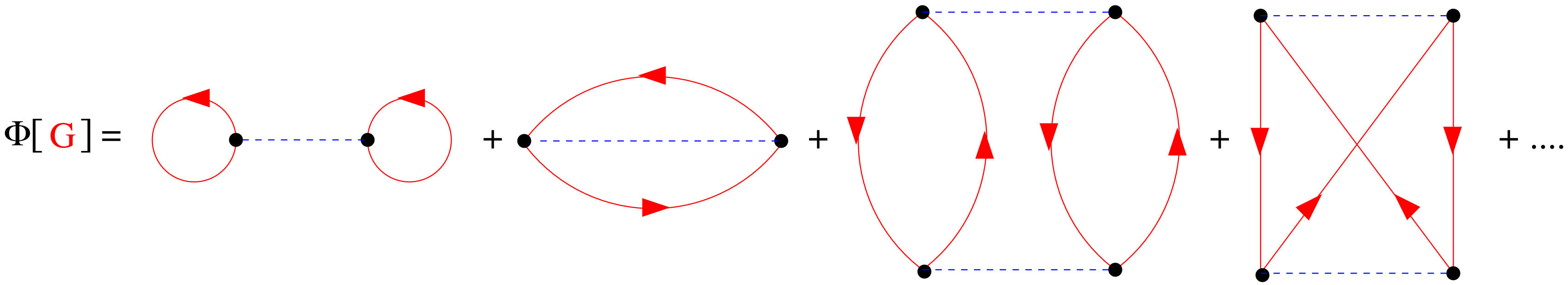
But: No way to calculate this for an interacting system of macroscopic size

The Grand Canconical Potential of interacting Fermions

Luttinger and Ward have derived an expression for the Grand Canonical Potential of interacting Fermions (J.M. Luttinger and J.C. Ward, Phys. Rev. **118**, 1417 (1960))

$$\Omega' = -\lim_{\eta \to 0^+} \frac{1}{\beta} \sum_{\mathbf{k},\nu} e^{i\omega_\nu \eta} \left[\ln \, \mathrm{det} \left(-\mathbf{G}^{-1}(\mathbf{k}, i\omega_\nu) \right) + \mathrm{trace} \left(\mathbf{G}(\mathbf{k}, i\omega_\nu) \, \mathbf{\Sigma}(\mathbf{k}, i\omega_\nu) \right) \right] + \Phi \, [\mathbf{G}].$$

- $\omega_\nu = \dfrac{(2\nu+1)\pi}{\hbar\beta}$: Matsubara Frequencies for $n_N = 1$
- $\mathbf{G}$: Green's Function, $\mathbf{\Sigma}$: Self-Energy
- $\Phi[\mathbf{G}]$: The Luttinger-Ward functional:



We now want to proove that $\Omega' = \Omega$ thereby following the original proof by Luttinger and Ward

- We replace $H \to H_0 + \lambda H_1$
- We show $\Omega' = \Omega$ for $\lambda = 0$ (the case of noninteracting electrons)
- We calculate $\lambda \partial_\lambda \, \Omega$
- We calculate $\lambda \partial_\lambda \, \Omega'$ and show that it is equal to $\lambda \partial_\lambda \, \Omega$

Obviously this prooves the equality of Ω' and Ω

The case $\lambda = 0$: Noninteracting Fermions

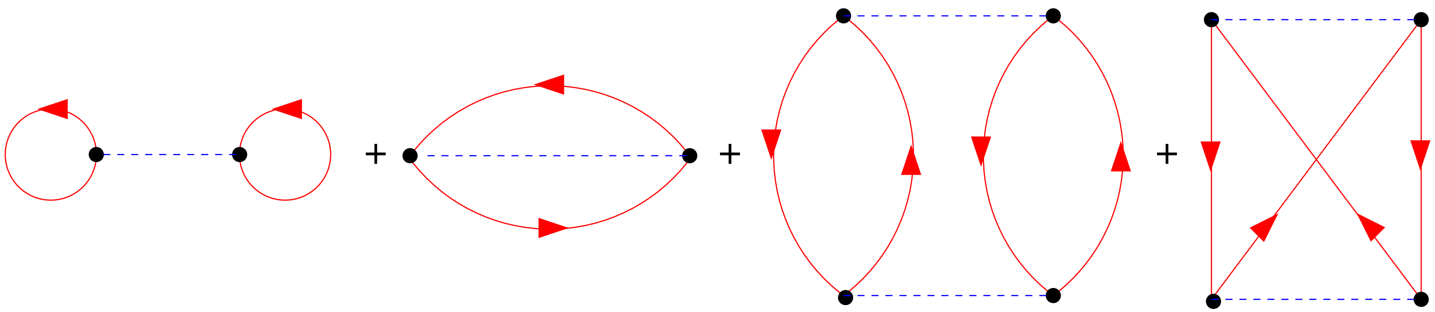
The Grand Canonical potential of free Bloch electrons is

$$\Omega \;=\; -\frac{1}{\beta}\;\sum_{n=1}^{2n_{orb}}\;\sum_{\mathbf{k}}\;\ln\left(1+e^{-\beta(E_n(\mathbf{k})-\mu)}\right)$$

The expression by Luttinger and Ward is

$$\Omega' \;=\; -\lim_{\eta\to 0^+}\frac{1}{\beta}\sum_{\mathbf{k},\nu} e^{i\omega_\nu\eta}\;\;\ln\,\mathbf{det}\left(-i\omega_\nu+\frac{\mathbf{t}(\mathbf{k})-\mu}{\hbar}\right)$$

For noninteracting electrons we have $\Sigma = 0$ and $\Phi = 0$:

$\Phi[\,G\,] =$  + ...

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- We calculate $\lambda \partial_\lambda \Omega$
- We calculate $\lambda \partial_\lambda \Omega'$ and show that it is equal to $\lambda \partial_\lambda \Omega$

Obviously this prooves the equality of Ω' and Ω

Calculation of $\lambda \frac{\partial \Omega}{\partial \lambda}$

The definition of Ω

$$\begin{aligned} \Omega &= -\frac{1}{\beta} \ln Z \\ &= -\frac{1}{\beta} \ln \left(\text{trace } e^{-\beta(H_0 + \lambda H_1 - \mu N)} \right) \end{aligned}$$

Here we use

$$\begin{aligned} \lambda \frac{\partial}{\partial \lambda} \Omega(\lambda) &= -\frac{1}{\beta} \lambda \frac{\partial}{\partial \lambda} \ln \left(\text{trace} \left(e^{-\beta(H_0 + \lambda H_1 - \mu N)} \right) \right) \\ &= \frac{1}{Z} \text{trace} \left(\lambda H_1 \, e^{-\beta(H_0 + \lambda H_1 - \mu N)} \right) \\ &= \langle \lambda H_1 \rangle_\lambda \end{aligned}$$

$\langle ... \rangle_\lambda$: thermal average *at interaction strength* λ

Calculation of $\langle \lambda H_1 \rangle_\lambda$

This can be obtained from the equation of motion of the Green's function

$$\langle \lambda H_1 \rangle_\lambda \;=\; -\frac{1}{2} \lim_{\tau \to 0^-} \sum_{\mathbf{k}} \text{trace} \left(\hbar \frac{\partial}{\partial \tau} + \mathbf{t}(\mathbf{k}) - \mu \right) \; \mathbf{G}_\lambda(\boldsymbol{k}, \tau),$$

Now: Use the Dyson equation

$$\left(i\omega_\nu - \frac{\mathbf{t}(\mathbf{k}) - \mu}{\hbar} - \boldsymbol{\Sigma}_\lambda(\mathbf{k}, i\omega_\nu) \right) \boldsymbol{G}_\lambda(\mathbf{k}, i\omega_\nu) \;=\; 1$$

Its Fourier transform is

$$\left(-\frac{\partial}{\partial \tau} - \frac{\mathbf{t}(\mathbf{k}) - \mu}{\hbar} \right) \boldsymbol{G}_\lambda(\mathbf{k}, \tau) - \int_0^{\beta\hbar} \boldsymbol{\Sigma}_\lambda(\mathbf{k}, \tau - \tau') \; \boldsymbol{G}_\lambda(\mathbf{k}, \tau') d\tau' \;=\; \delta(\tau)$$

$$\left(-\frac{1}{\hbar} \right) \; \left(\hbar \frac{\partial}{\partial \tau} + \mathbf{t}(\mathbf{k}) - \mu \right) \boldsymbol{G}_\lambda(\mathbf{k}, \tau) - \int_0^{\beta\hbar} \boldsymbol{\Sigma}_\lambda(\mathbf{k}, \tau - \tau') \; \boldsymbol{G}_\lambda(\mathbf{k}, \tau') d\tau' \;=\; \delta(\tau)$$

Using $\lim_{\tau \to 0^-} \delta(\tau) = 0$:

$$\left(\hbar \frac{\partial}{\partial \tau} + \mathbf{t}(\mathbf{k}) - \mu \right) \boldsymbol{G}_\lambda(\mathbf{k}, \tau) \;=\; -\hbar \int_0^{\beta\hbar} \boldsymbol{\Sigma}_\lambda(\mathbf{k}, \tau - \tau') \; \boldsymbol{G}_\lambda(\mathbf{k}, \tau') d\tau'$$

Calculation of $\langle \lambda H_1 \rangle_\lambda$

This can be obtained from the equation of motion of the Green's function

$$\langle \lambda H_1 \rangle_\lambda \;=\; -\frac{1}{2} \lim_{\tau \to 0^-} \sum_{\mathbf{k}} \text{trace} \left(\hbar \frac{\partial}{\partial \tau} + \mathbf{t}(\mathbf{k}) - \mu \right) \mathbf{G}_\lambda(\boldsymbol{k}, \tau),$$

We found....

$$\left(\hbar \frac{\partial}{\partial \tau} - \mu + \mathbf{t}(\mathbf{k}) \right) \boldsymbol{G}_\lambda(\mathbf{k}, \tau) \;=\; -\hbar \int_0^{\beta\hbar} \boldsymbol{\Sigma}_\lambda(\mathbf{k}, \tau - \tau') \, \boldsymbol{G}_\lambda(\mathbf{k}, \tau') d\tau'$$

$$= \; -\hbar \frac{1}{\beta\hbar} \sum_\nu \; e^{-i\omega_\nu \tau} \, \boldsymbol{\Sigma}_\lambda(\boldsymbol{k}, i\omega_\nu) \, \boldsymbol{G}_\lambda(\boldsymbol{k}, i\omega_\nu)$$

... so that the end result is (remember that $\tau \to 0^-$)

$$\lambda \frac{\partial}{\partial \lambda} \Omega(\lambda) = \langle \lambda H_1 \rangle_\lambda \;=\; \frac{1}{2\beta} \sum_{\mathbf{k},\nu} \text{trace} \, \boldsymbol{\Sigma}_\lambda(\boldsymbol{k}, i\omega_\nu) \, \boldsymbol{G}_\lambda(\boldsymbol{k}, i\omega_\nu)$$

We now want to proove that $\Omega' = \Omega$ thereby following the original proof by Luttinger and Ward:

- We replace $H \to H_0 + \lambda H_1$
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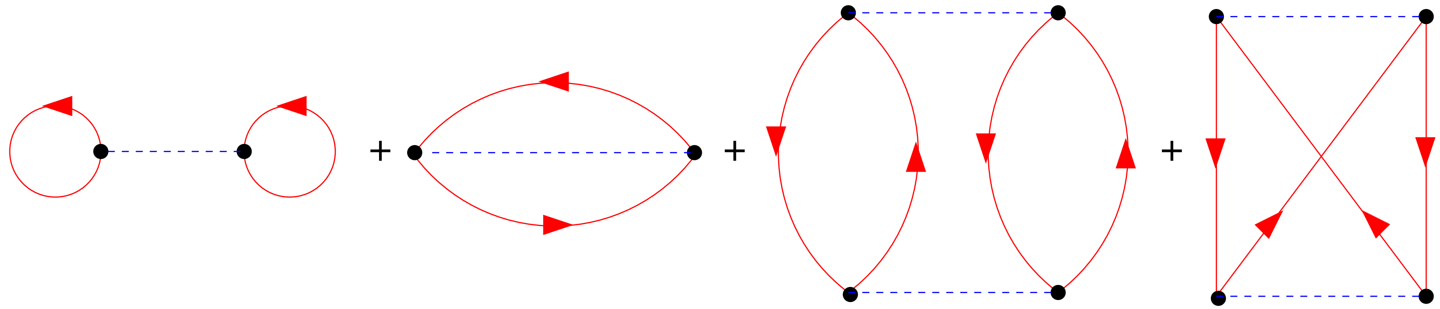
Obviously this prooves the equality of Ω' and Ω

The Precise Definition and Properties of the Luttinger-Ward Functional $\Phi[\mathbf{G}]$

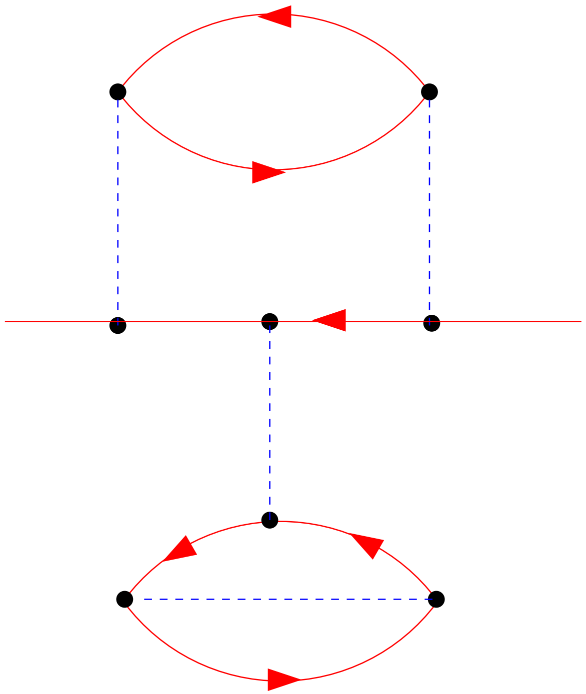
Reminder: The Luttinger-Ward functional is defined in terms of Feynman diagrams

$\Phi[\,G\,] =$  + ...

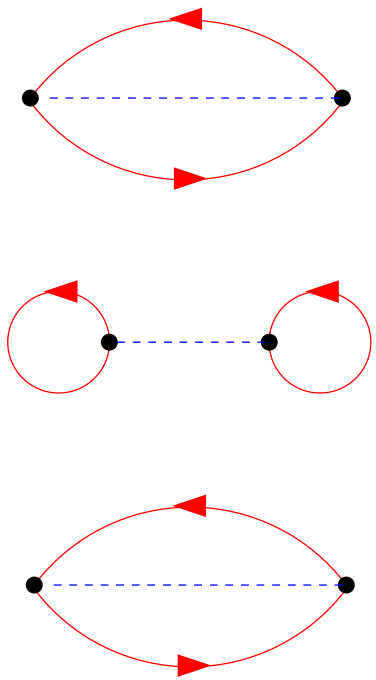
The diagrams which are included into Φ are

- Closed (no open ends)
- Connected (no subdiagrams with no lines connecting them)
- Skeleton diagrams (no self-energy parts in any Green's function line)

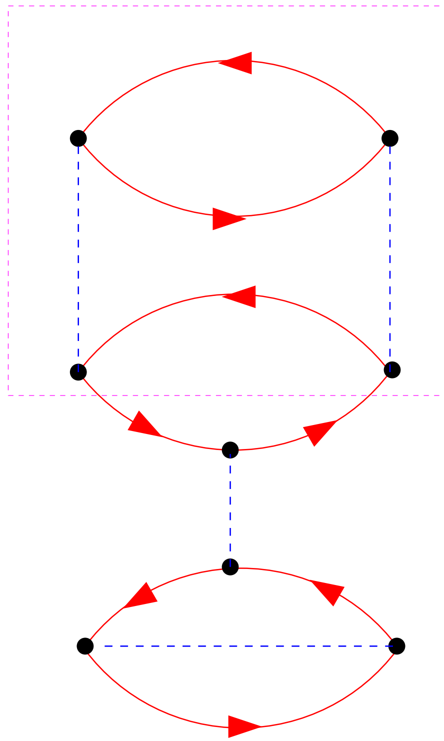
Excluded diagrams



Open ends!

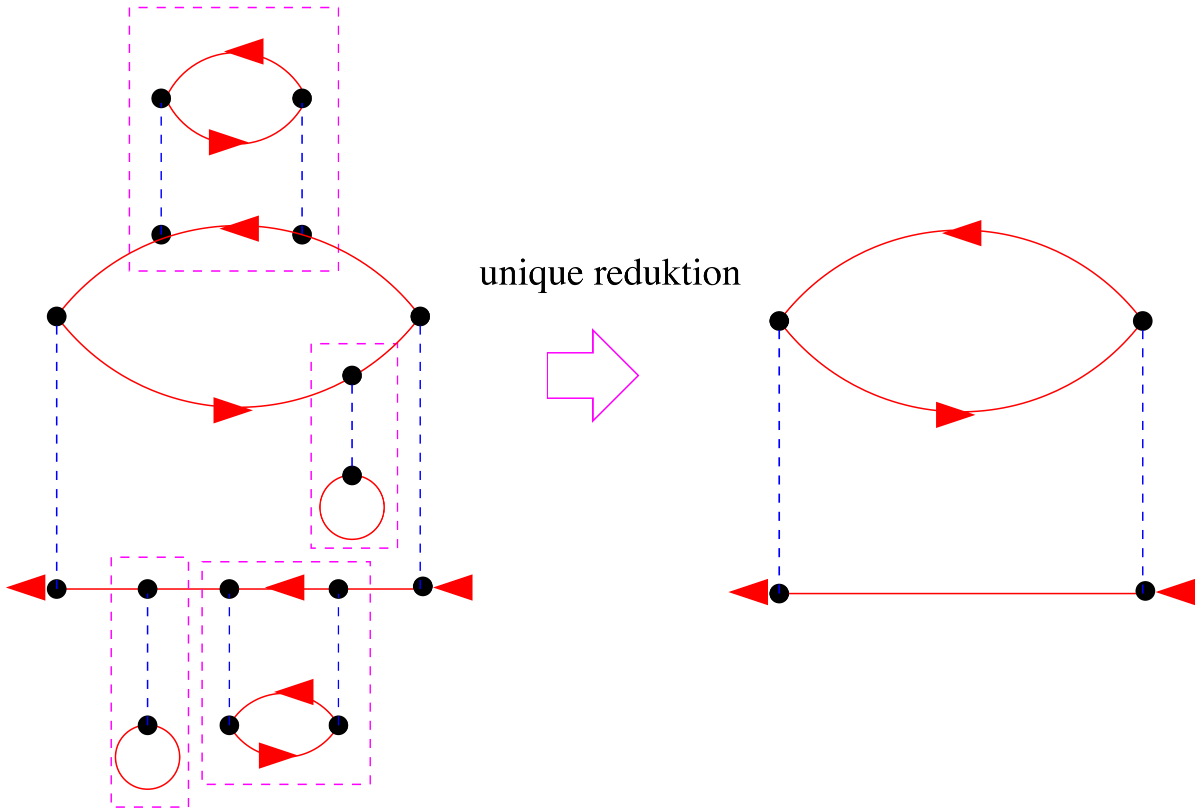


Disconnected!



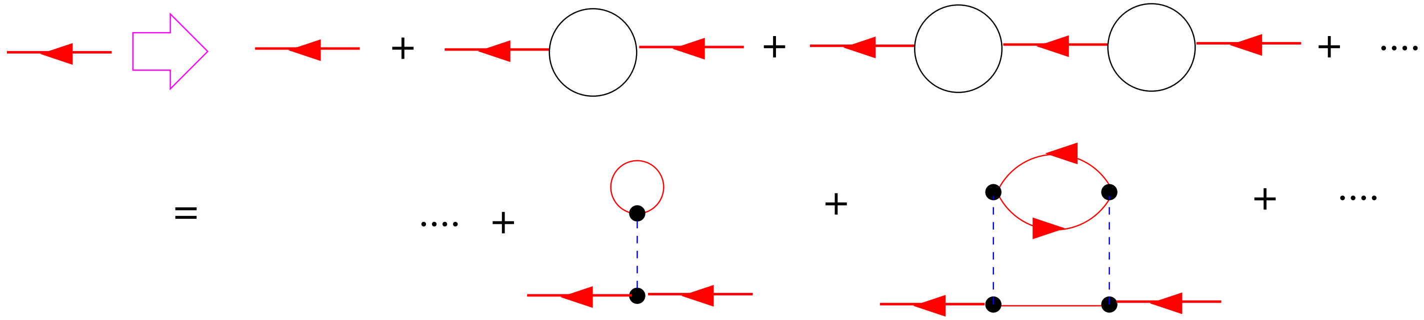
Self–energy insertion!

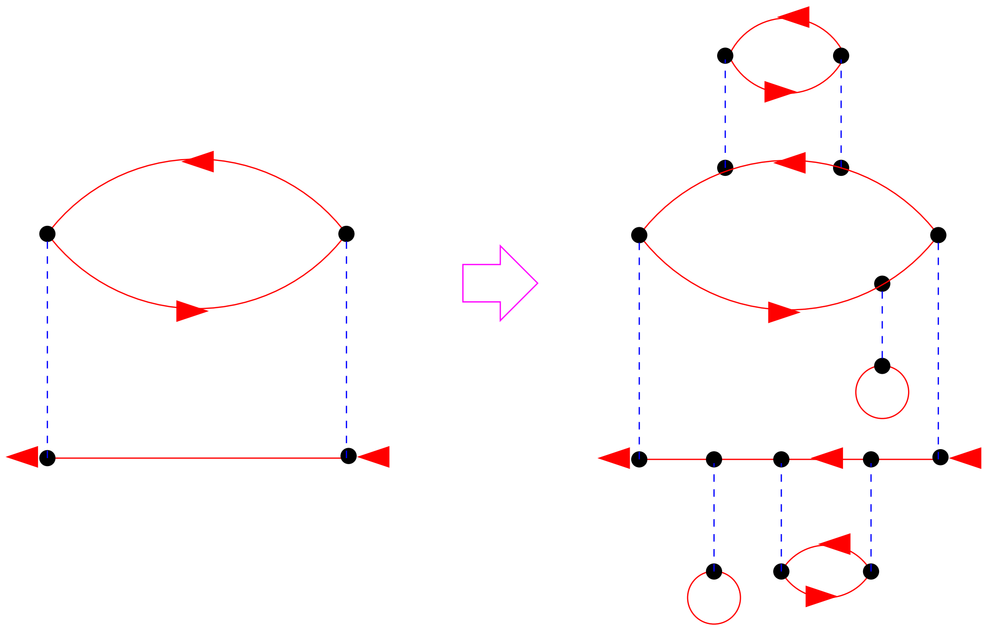
Short disgression: Self-energy diagrams can be reduced uniquely to skeleton diagrams



Each self-energy diagram can be reduced uniquely to a skeleton diagram by removing all self-energy insertions

This also goes the other way round

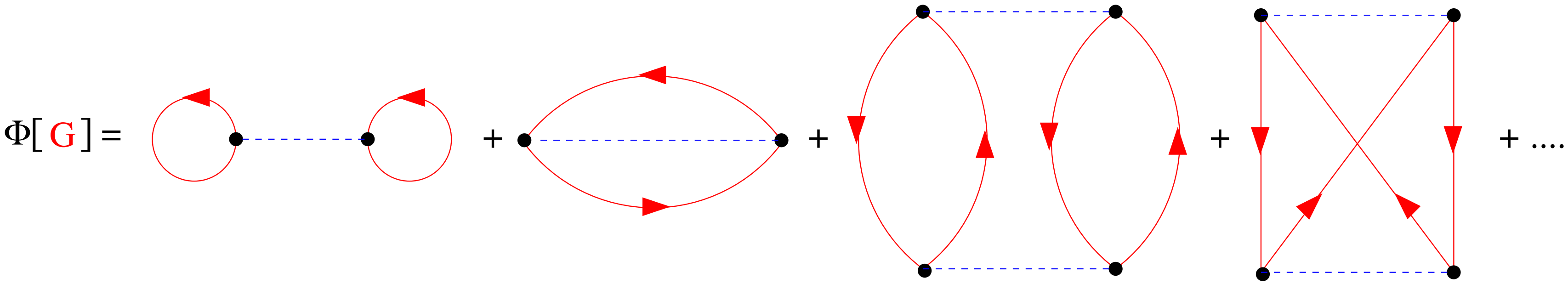




By drawing all skeleton-diagrams for the self-energy and 'translating' Green's function lines into the full Green's function instead of the noninteracting one the total self-energy is obtained

The Precise Definition and Properties of the Luttinger-Ward Functional $\Phi[\mathbf{G}]$

Reminder: The Luttinger-Ward functional is defined in terms of Feynman diagrams



The diagrams which are included into Φ are

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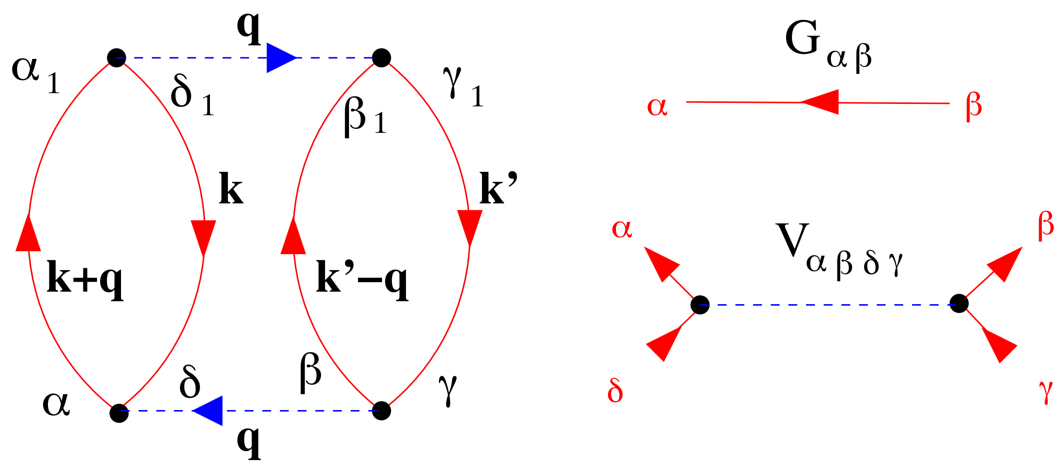
- Connected (no subdiagrams with no lines connecting them)
- Skeleton diagrams (no self-energy parts in any Green's function line)

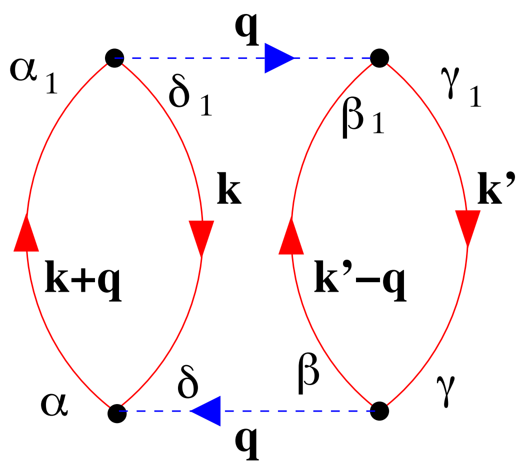
The Diagrams are Converted into Multiple Sums using the Standard Feynman Rules....

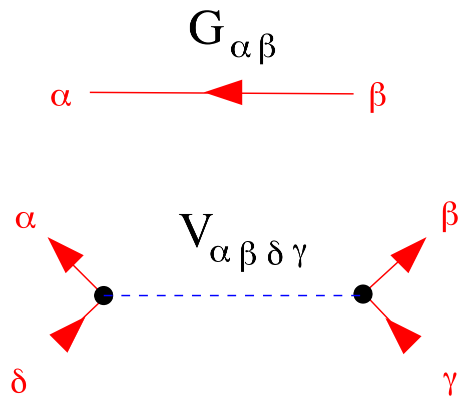


$$\left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma,\delta} \sum_{\alpha_1,\beta_1,\gamma_1,\delta_1} \sum_{\nu,\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{q},-\mathbf{q})$$

$$G_{\alpha_1,\alpha}(\mathbf{k}+\mathbf{q}, i\omega_\nu + \omega_\mu)\, G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu)\, G_{\beta_1,\beta}(\mathbf{k}'-\mathbf{q}, i\omega_{\nu'} - i\omega_\mu)\, G_{\gamma,\gamma_1}(\mathbf{k}', i\omega_{\nu'})$$

.... but there is one crucial difference!



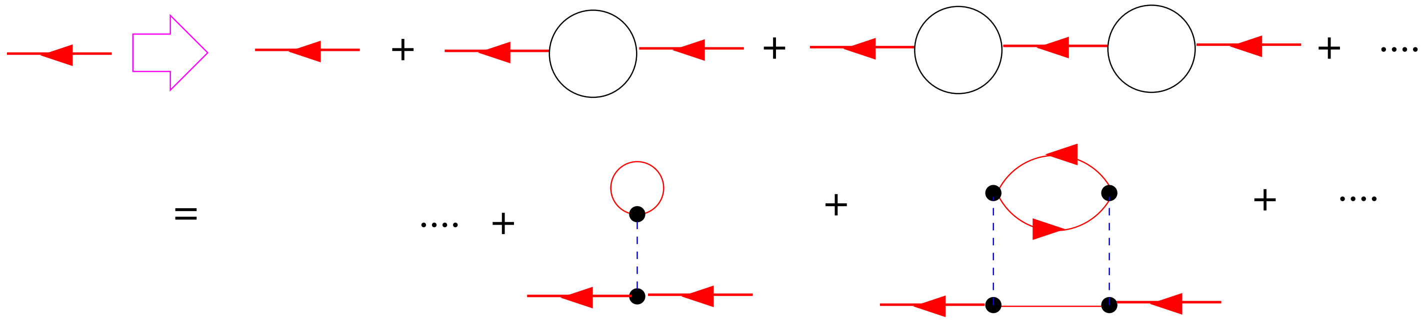


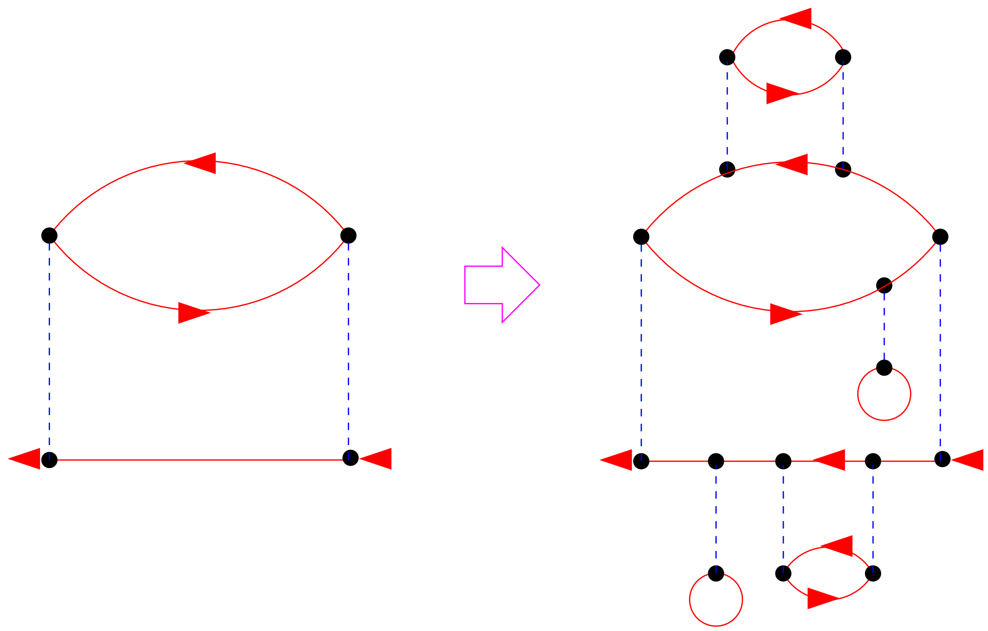
$$\left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma,\delta} \sum_{\alpha_1,\beta_1,\gamma_1,\delta_1} \sum_{\nu,\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q})\ V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{q},-\mathbf{q})$$

$$G_{\alpha_1,\alpha}(\mathbf{k}+\mathbf{q}, i\omega_\nu+\omega_\mu)\ G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu)\ G_{\beta_1,\beta}(\mathbf{k}'-\mathbf{q}, i\omega_{\nu'}-i\omega_\mu)\ G_{\gamma,\gamma_1}(\mathbf{k}', i\omega_{\nu'})$$

The Green's function in the algebraic expression corresponding to a given diagram is *not* the noninteracting Green's function $\boldsymbol{G}^{(0)}$ but the Green's function $\boldsymbol{G}$ which is the argument of the functional: $\Phi[\boldsymbol{G}]$!

Reminder: using the full Green's function instead of the noninteracting one is precisely the same idea as in the skeleton-diagram expansion of the self-energy!





Symmetry factors

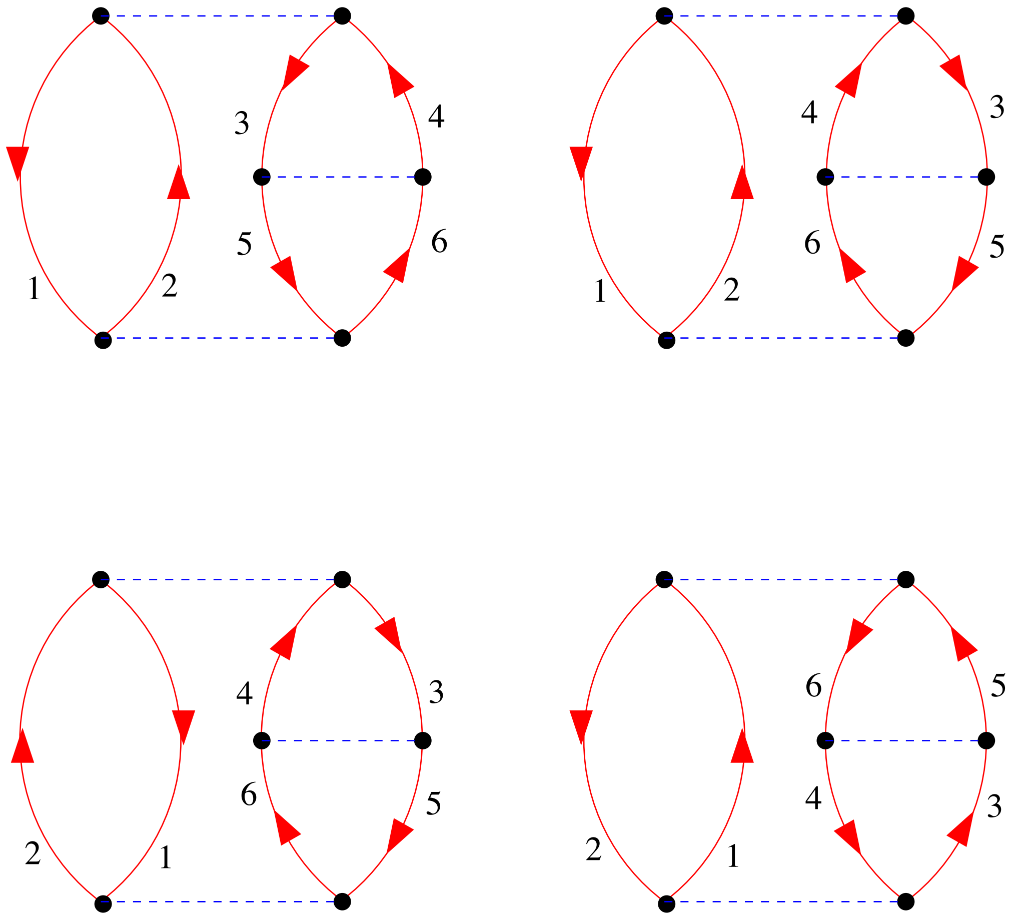
In addition to the factors from the Feynman rules the expression for each diagram is multiplied by

$$-\frac{1}{\beta S}$$

where the integer S is the symmetry factor of the diagram

In simplest terms S gives the number of ways in which the diagram can be 'deformed' such that it is identical to itself

Example

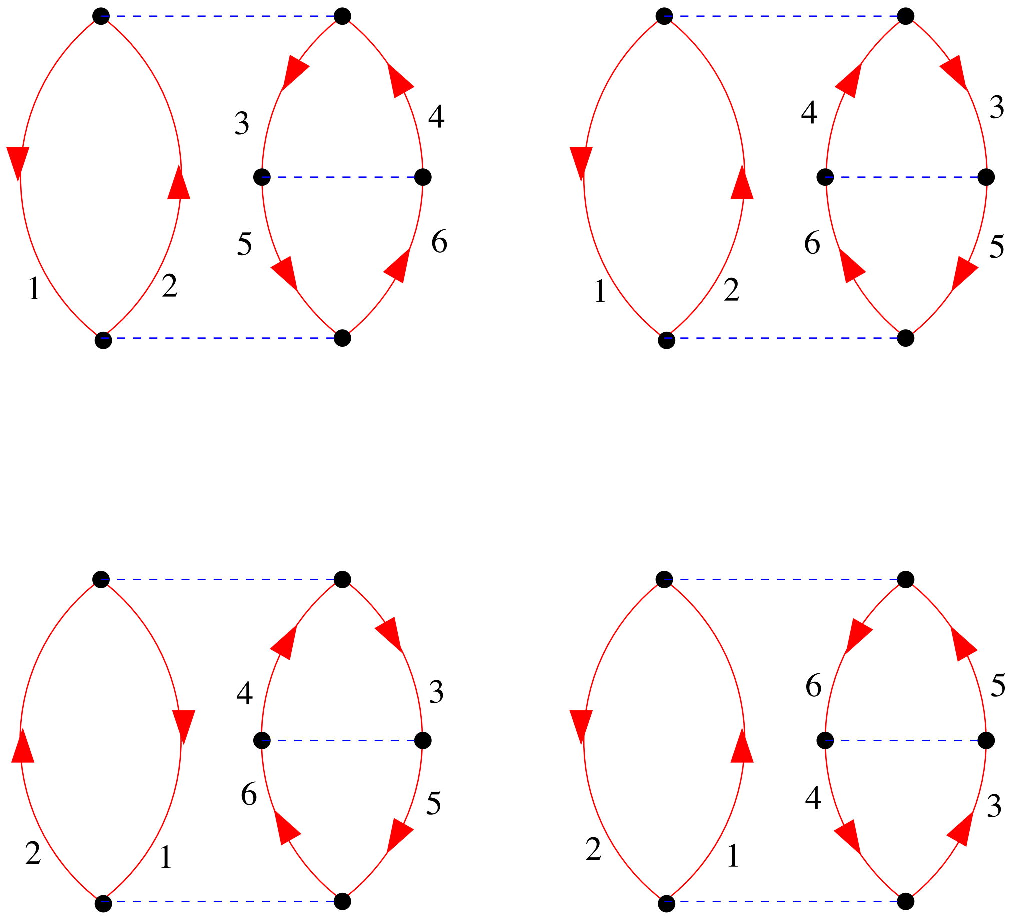


The final diagram looks exactly like the original one - including direction of all arrows - but the Green's function lines are permuted!

Determination of the Symmetry Factors S

- We label the lines on the diagram by integers $\in \{1 \ldots n\}$
- We imagine that the diagram can be 'taken off the paper' and is completely flexible
- We deform the diagram but without breaking any line or changing the direction of any arrow on a Green's function line - this means we maintain the connectivity properties of the diagram
- If the resulting diagram looks exactly the same as the original one but with permuted labels we call this a symmetry operation of the diagram
- The symmetry factor S of a diagram is the number of different symmetry operations (including the 'unit deformation')
- All Green's function lines then can be grouped into classes such that the members of a class are permuted amongst themselves
- If two lines i and j belong to the same class the diagram can be deformed such that it looks completely the same but i and j have switched their positions
- We call all lines of a class symmetry equivalent

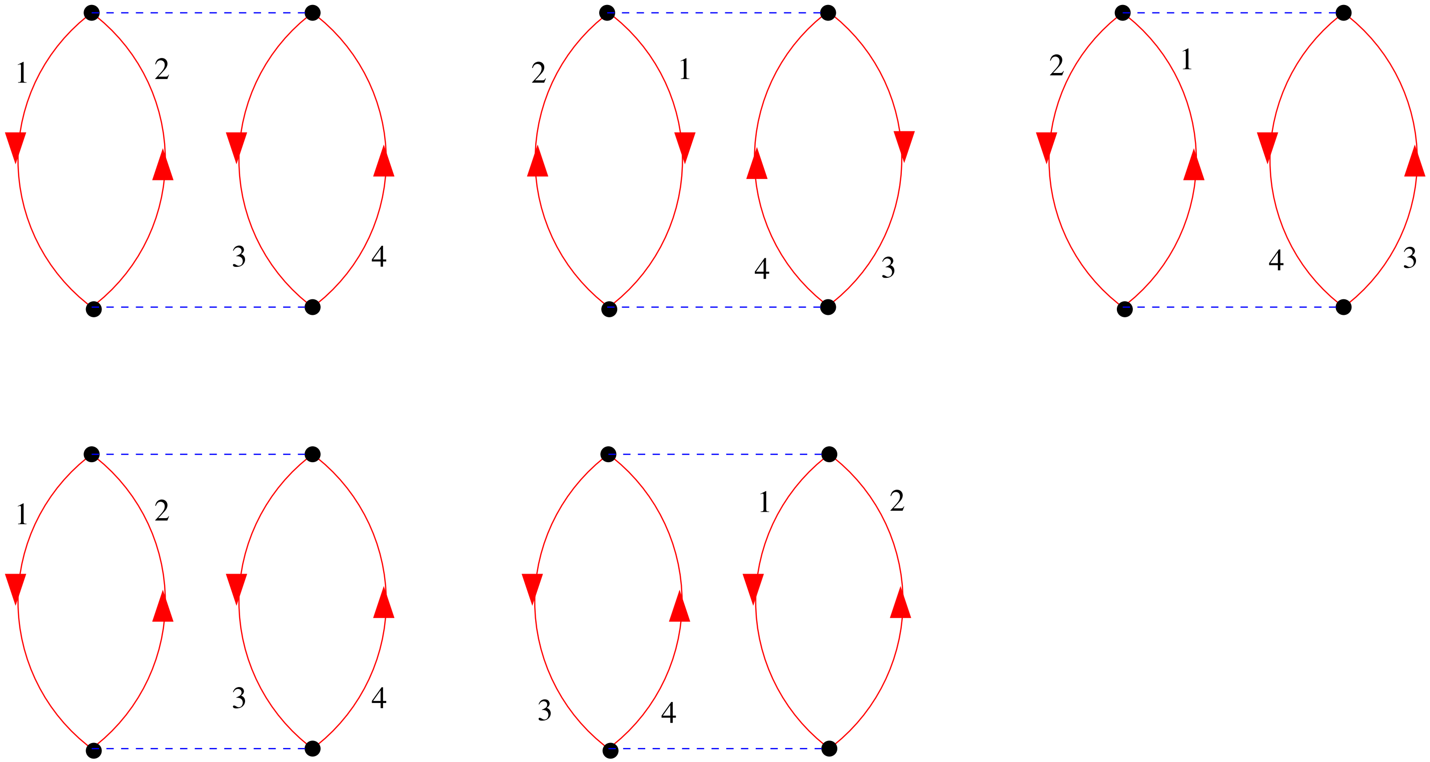
Example



For this diagram there are no further symmetry operations $\rightarrow$ the diagram has $S = 2$ (we include identity!)

The classes of equivalent Green's function lines are $(1, 2)$, $(3, 6)$ and $(4, 5)$

<u>Another example</u>



Above we show two symmetry operations corresponding to the permutations $(2, 1, 4, 3)$ and $(3, 4, 1, 2)$ - there is a third operation corresponding to the product of these two permutations namely $(4, 3, 2, 1) \rightarrow$ the diagram has $S = 4$, there is only one class comprising all lines

Further discussion

- An n^{th} order diagram - i.e. a diagram with n interaction lines - has $2n$ Green's function lines
- Assume that the diagram has symmetry factor S
- This means the classes of equivalent Green's function have S members each
- The number of classes - therefore is $\frac{2n}{S}$ (which of course better be an integer...)
- If two lines - say i and j - belong to the same class it means that the diagram can be redrawn such that it looks completely the same but with line j in place of line i

The real defining property of the Luttinger-Ward functional

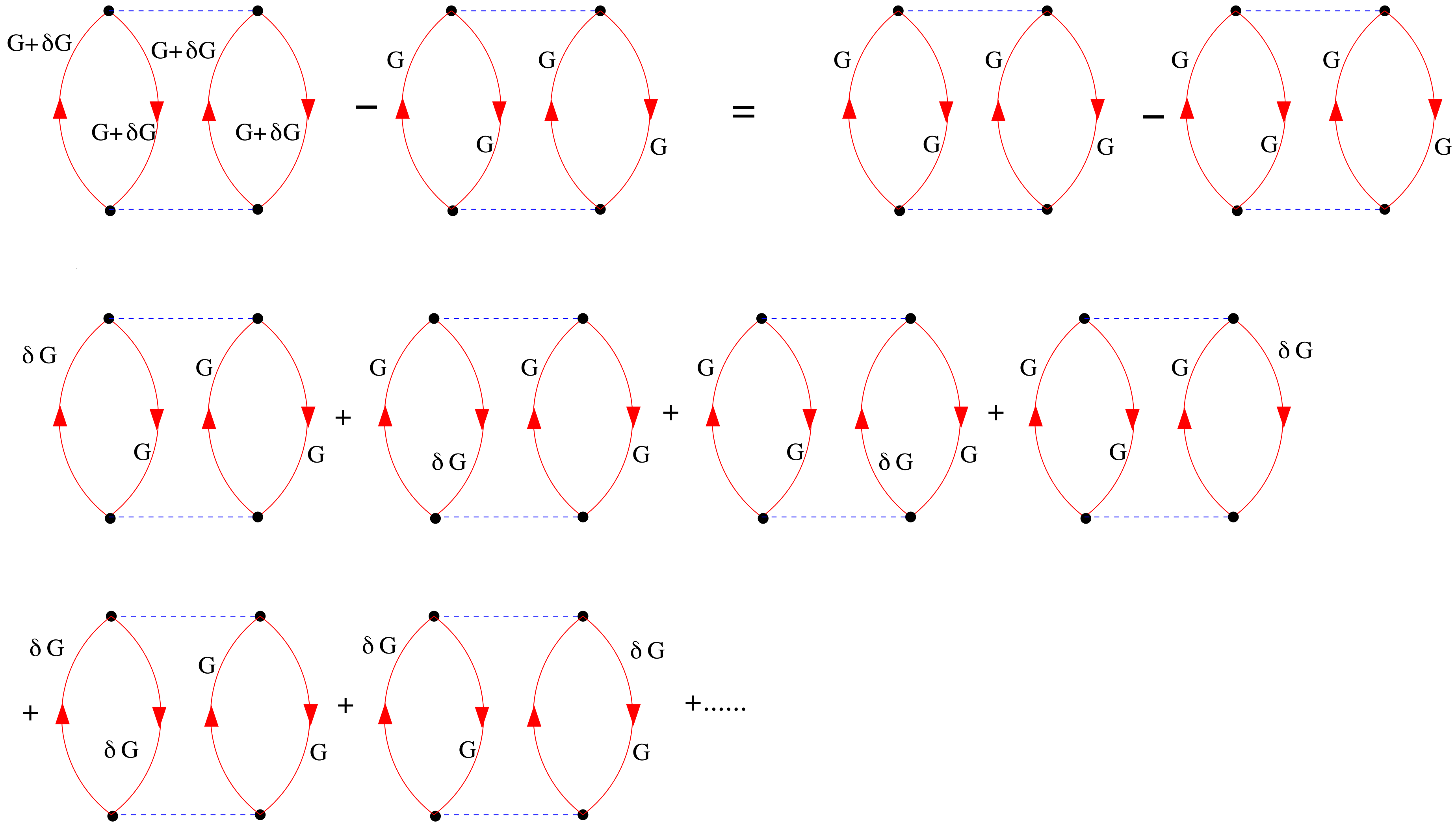
The Luttinger-Ward functional is the generating functional of the self-energy

$$\frac{\partial \Phi[\boldsymbol{G}]}{\partial G_{\alpha,\beta}(\mathbf{k}, i\omega_\nu)} = \frac{1}{\beta}\,\Sigma_{\beta,\alpha}(\mathbf{k}, i\omega_\nu)$$

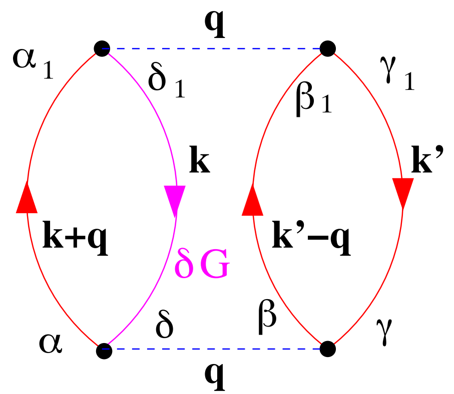
To see this we need to consider the change of a given diagram contributing to Φ under a change of G:

$$G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) \rightarrow G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) + \delta G_{\alpha\beta}(\mathbf{k}, i\omega_\nu)$$

Let us consider the variation of Φ under a variation $G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) \to G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) + \delta G_{\alpha\beta}(\mathbf{k}, i\omega_\nu)$



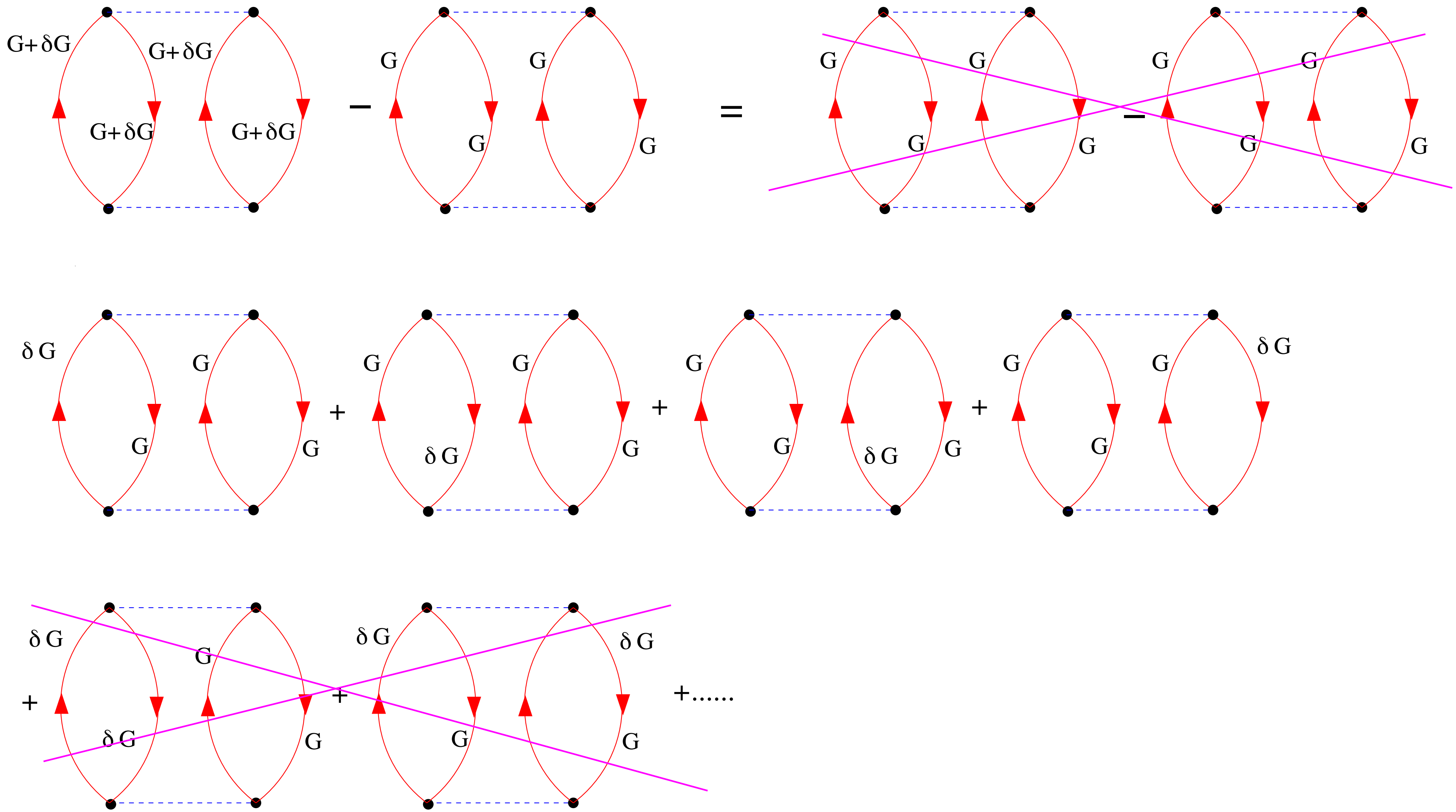
What is the meaning of the 'substituted' diagrams?



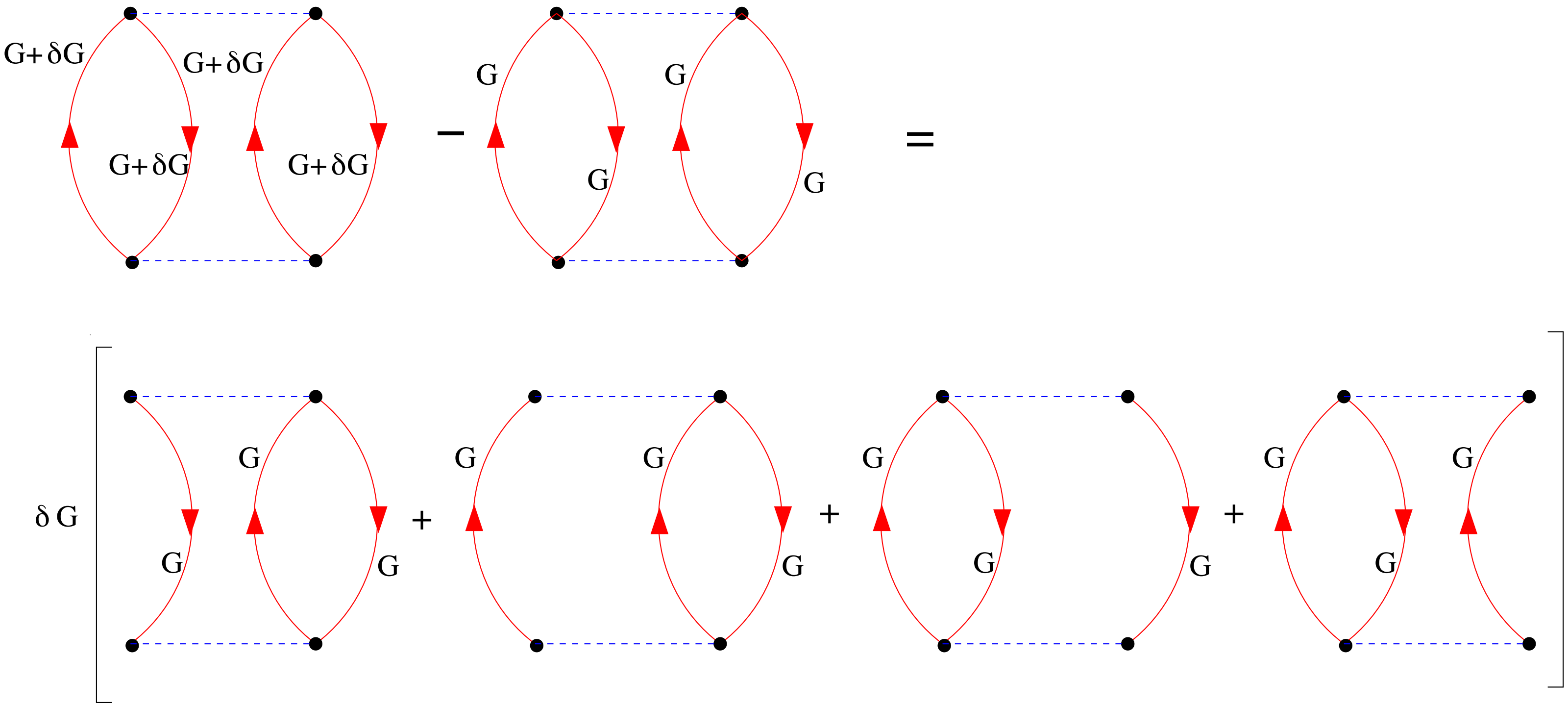
$$\left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma,\delta} \sum_{\alpha_1,\beta_1,\gamma_1,\delta_1} \sum_{\nu,\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{q},-\mathbf{q})$$

$$G_{\alpha_1,\alpha}(\mathbf{k}+\mathbf{q}, i\omega_\nu + \omega_\mu)\, \delta G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu)\, G_{\beta_1,\beta}(\mathbf{k}'-\mathbf{q}, i\omega_{\nu'} - i\omega_\mu)\, G_{\gamma,\gamma_1}(\mathbf{k}', i\omega_{\nu'})$$

Let us consider the variation of Φ under a variation $G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) \to G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) + \delta G_{\alpha\beta}(\mathbf{k}, i\omega_\nu)$



Let us consider the variation of Φ under a variation $G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) \to G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) + \delta G_{\alpha\beta}(\mathbf{k}, i\omega_\nu)$

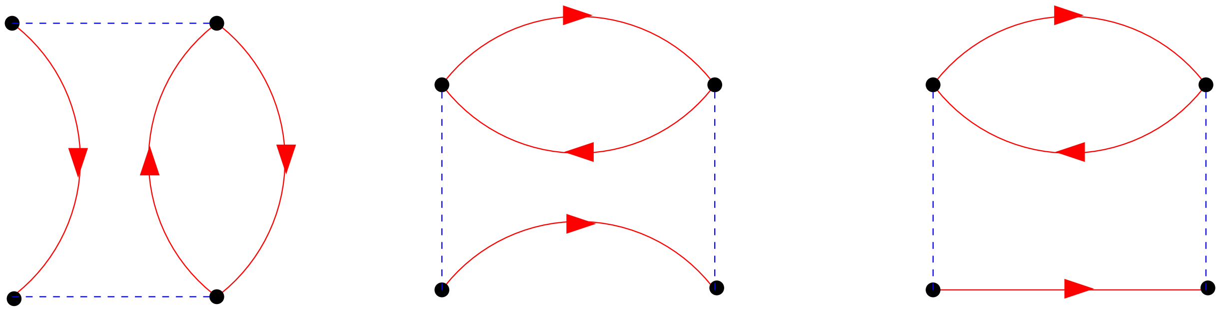


Forming the derivative

$$\frac{\partial \Phi}{\partial G_{\alpha,\beta}(\mathbf{k}, i\omega_\nu)}$$

means 'opening' one of the Green's function lines in the diagrams contributing to Φ

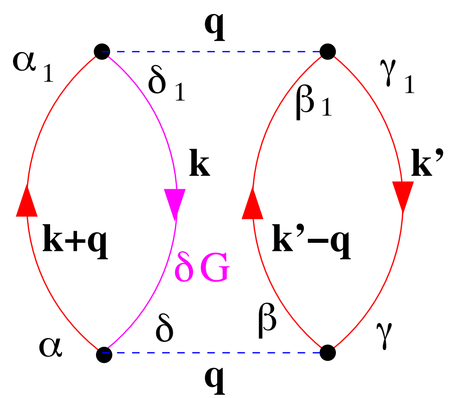
The 'opened' diagrams then indeed 'look like' self-energy diagrams:



The question is: Do we have the correct prefactors so as to fulfill

$$\frac{\partial \Phi}{\partial G_{\alpha,\beta}(\mathbf{k}, i\omega_\nu)} = \frac{1}{\beta}\, \Sigma_{\beta,\alpha}(\mathbf{k}, i\omega_\nu)\ ?$$

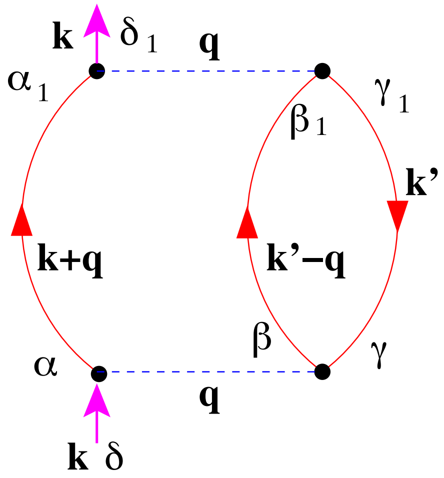
Factoring out the variation δG 'fixes' the momentum, frequency and band indices of the remaining diagram



$$\left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma,\delta} \sum_{\alpha_1,\beta_1,\gamma_1,\delta_1} \sum_{\nu,\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{q},-\mathbf{q})$$

$$G_{\alpha_1,\alpha}(\mathbf{k}+\mathbf{q}, i\omega_\nu + \omega_\mu)\, \delta G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu)\, G_{\beta_1,\beta}(\mathbf{k}'-\mathbf{q}, i\omega_{\nu'} - i\omega_\mu)\, G_{\gamma,\gamma_1}(\mathbf{k}', i\omega_{\nu'})$$

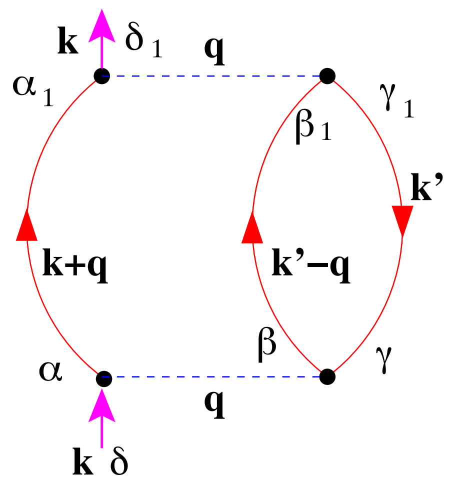
Factoring out the variation δG 'fixes' the momentum, frequency and band indices of the remaining diagram



$$\delta G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu) \left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma} \sum_{\alpha_1,\beta_1,\gamma_1} \sum_{\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q}) \, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{q},-\mathbf{q})$$

$$G_{\alpha_1,\alpha}(\mathbf{k}+\mathbf{q}, i\omega_\nu + \omega_\mu) \qquad G_{\beta_1,\beta}(\mathbf{k}'-\mathbf{q}, i\omega_{\nu'} - i\omega_\mu) \, G_{\gamma,\gamma_1}(\mathbf{k}', i\omega_{\nu'})$$

Factoring out the variation δG 'fixes' the momentum, frequency and band indices of the remaining diagram

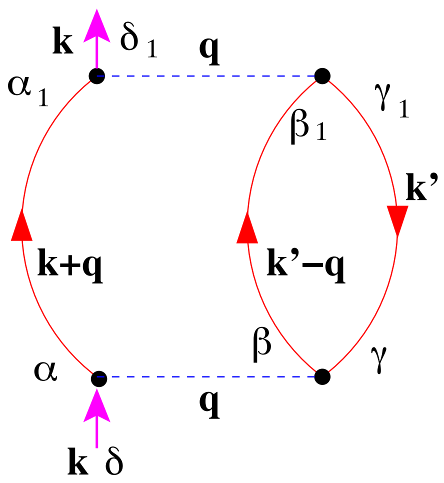


$$\color{magenta}{\delta G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu)} \left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma} \sum_{\alpha_1,\beta_1,\gamma_1} \sum_{\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{q},-\mathbf{q})$$

$$G_{\alpha_1,\alpha}(\mathbf{k}+\mathbf{q}, i\omega_\nu+\omega_\mu)\, G_{\beta_1,\beta}(\mathbf{k}'-\mathbf{q}, i\omega_{\nu'}-i\omega_\mu)\, G_{\gamma,\gamma_1}(\mathbf{k}', i\omega_{\nu'})$$

- The incoming and outgoing momentum and frequency are $\mathbf{k}$ and ω_ν
- There is still momentum/frequency conservation at each vertex and all remaining momenta, frequencies, band indices keep on being summed over - exactly as in the true expression for $\Sigma(\boldsymbol{k}, \omega)$

Factoring out the variation δG 'fixes' the momentum, frequency and band indices of the remaining diagram

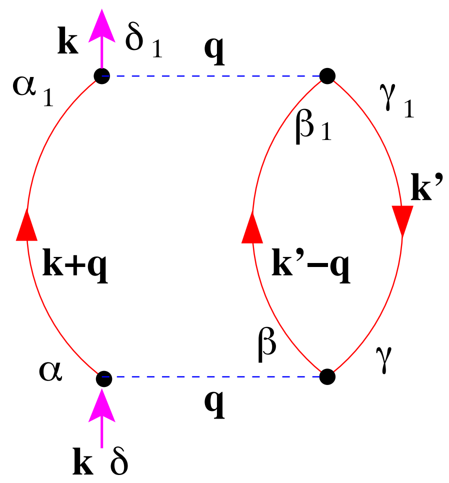


$$\textcolor{magenta}{\delta G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu)} \left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma} \sum_{\alpha_1,\beta_1,\gamma_1} \sum_{\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{q},-\mathbf{q})$$

$$G_{\alpha_1,\alpha}(\mathbf{k}+\mathbf{q}, i\omega_\nu + \omega_\mu)\, G_{\beta_1,\beta}(\mathbf{k}'-\mathbf{q}, i\omega_{\nu'} - i\omega_\mu)\, G_{\gamma,\gamma_1}(\mathbf{k}', i\omega_{\nu'})$$

- The remaining diagram has band index δ on its incoming entry and δ_1 on its outgoing entry
- This is exactly as in the true expression for $\Sigma_{\delta_1,\delta}(\boldsymbol{k},\omega)$

Factoring out the variation δG 'fixes' the momentum, frequency and band indices of the remaining diagram



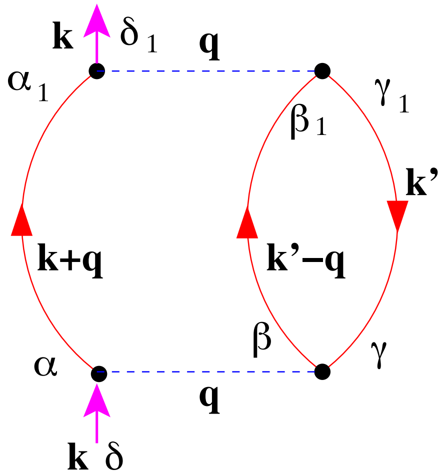
$$\delta G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu) \left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma} \sum_{\alpha_1,\beta_1,\gamma_1} \sum_{\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{q},-\mathbf{q})$$

$$G_{\alpha_1,\alpha}(\mathbf{k}+\mathbf{q}, i\omega_\nu + \omega_\mu)\, G_{\beta_1,\beta}(\mathbf{k}'-\mathbf{q}, i\omega_{\nu'} - i\omega_\mu)\, G_{\gamma,\gamma_1}(\mathbf{k}', i\omega_{\nu'})$$

- The order n (number of interaction lines) is not changed by opening a Fermion line

$$\left(\frac{-1}{\beta\hbar^2 N}\right)^n \text{ remains correct}$$

Factoring out the variation δG 'fixes' the momentum, frequency and band indices of the remaining diagram



$$\delta G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu) \left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma} \sum_{\alpha_1,\beta_1,\gamma_1} \sum_{\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{q},-\mathbf{q})$$

$$G_{\alpha_1,\alpha}(\mathbf{k}+\mathbf{q}, i\omega_\nu+\omega_\mu)\, G_{\beta_1,\beta}(\mathbf{k}'-\mathbf{q}, i\omega_{\nu'}-i\omega_\mu)\, G_{\gamma,\gamma_1}(\mathbf{k}', i\omega_{\nu'})$$

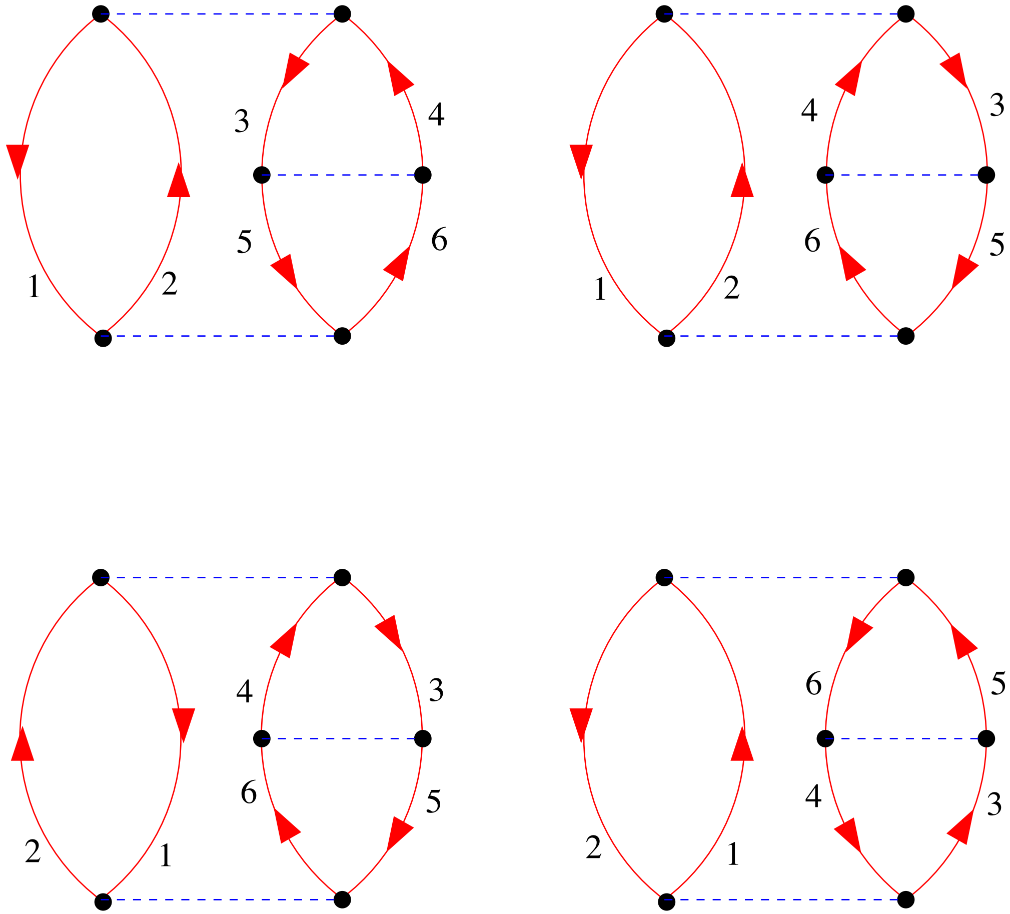
- Opening one Green's function lines reduces the number of Fermion loops F by 1 $\rightarrow$ the factor $(-1)^F$ changes sign - the extra (-1) in the prefactor takes care of this:

$$-\frac{1}{\beta S}$$

What about the factor $1/S$?

- Let us consider an n^{th} order Φ-diagram with symmetry factor S
- The symmetry factor S was the number of ways in which the diagram could be deformed into itself
- Then there are $2n/S$ classes, each containing S Green's function lines, which are symmetry equivalent to each other
- Symmetry equivalence means that the diagram can be deformed such that it looks exactly the same but with the two symmetry equivalent Green's function exchanged
- This means that if two symmetry equivalent lines are opened the resulting self-energy diagrams also can be deformed into each other and thus are completely identical
- All S Green's function lines in one class therefore give exactly the same self-energ diagram when they are opened
- Since we have $2n/S$ classes with S lines in each class the Φ-diagram gives $2n/S$ Σ-diagrams and each is produced S times
- This factor of S exactly cancels the factor of $1/S$ in the prefactor of the diagram

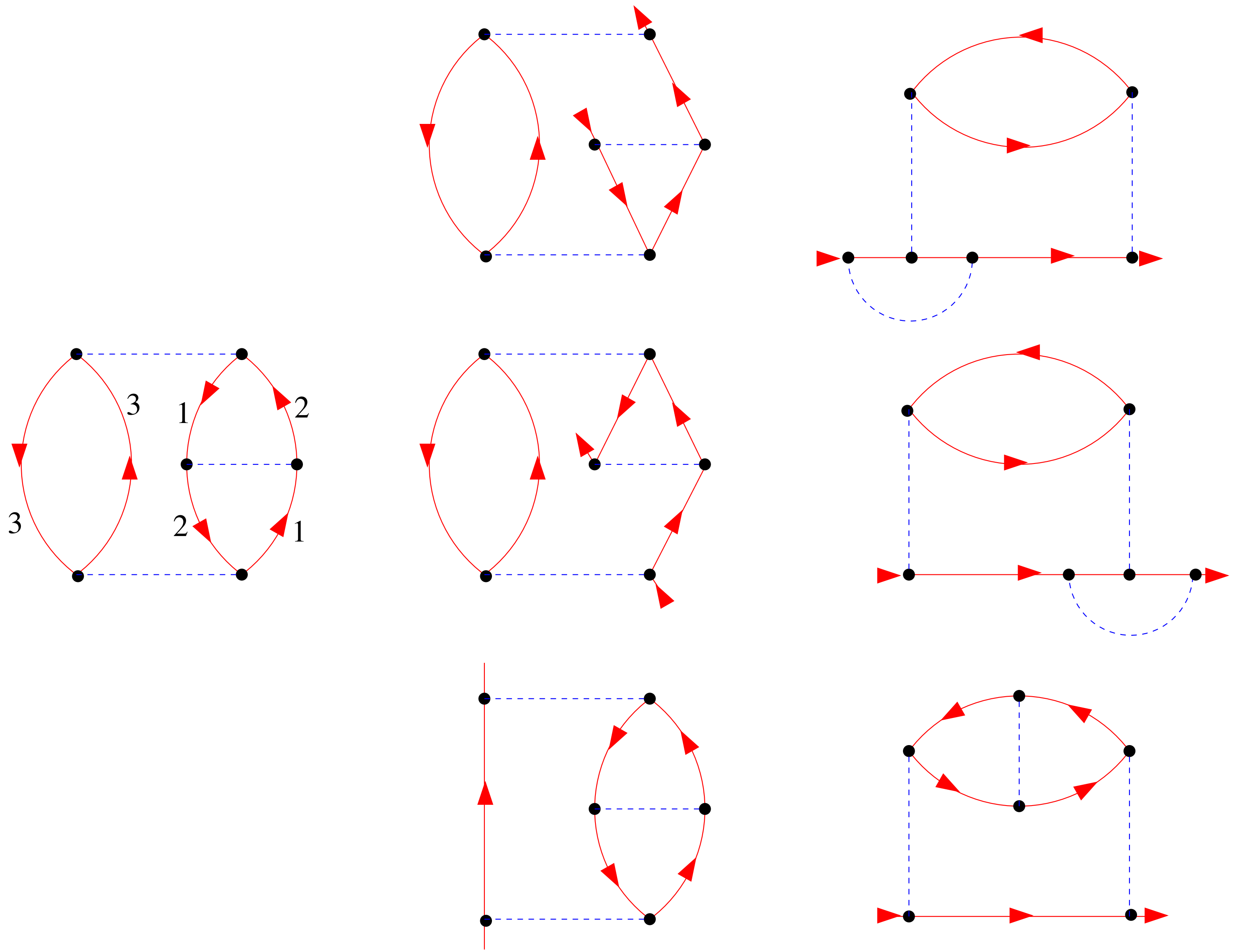
Example



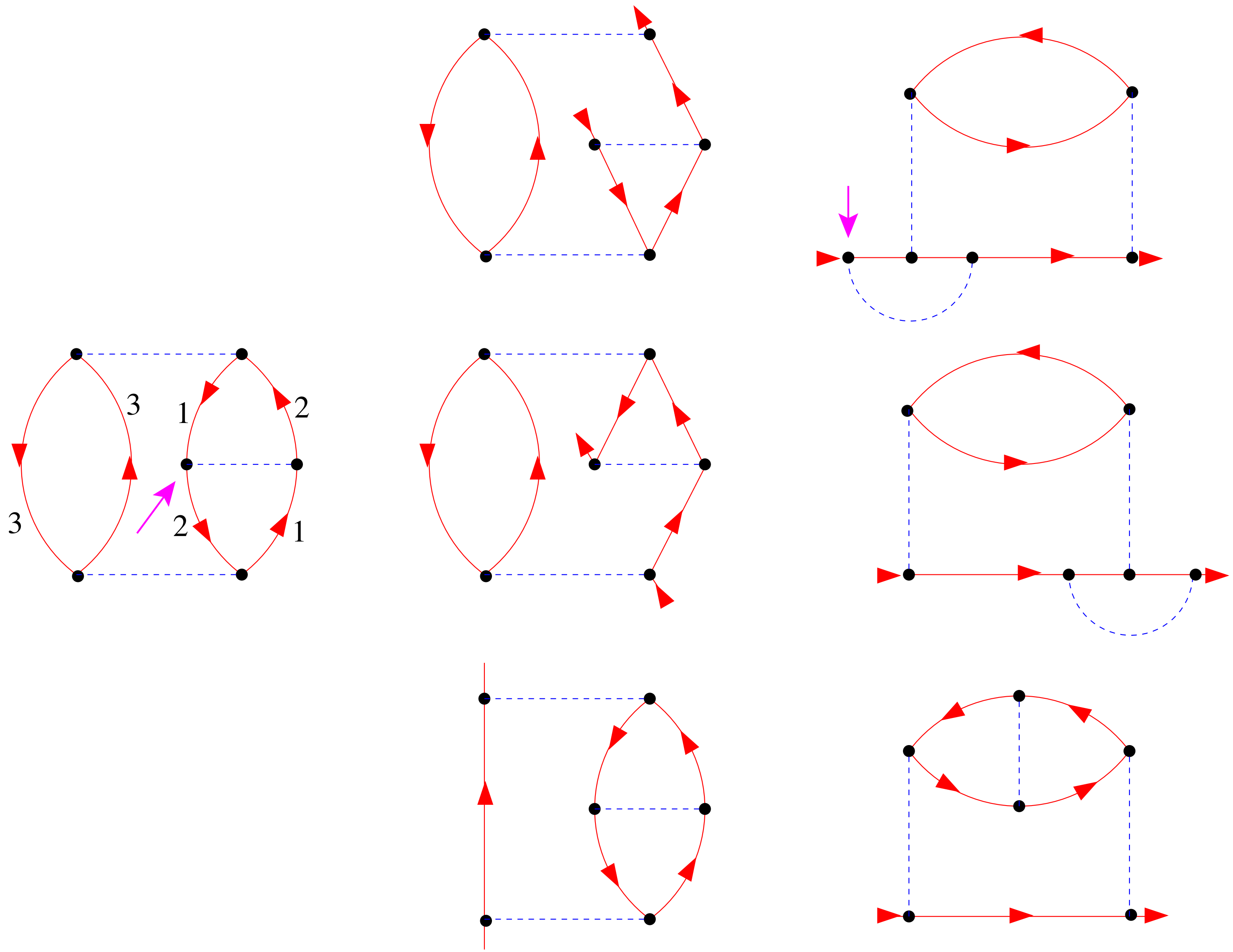
For this diagram there are no further symmetry operations $\rightarrow$ the diagram has $S = 2$ (we include identity!)

The classes of equivalent Green's function lines are $(1, 2)$, $(3, 6)$ and $(4, 5)$

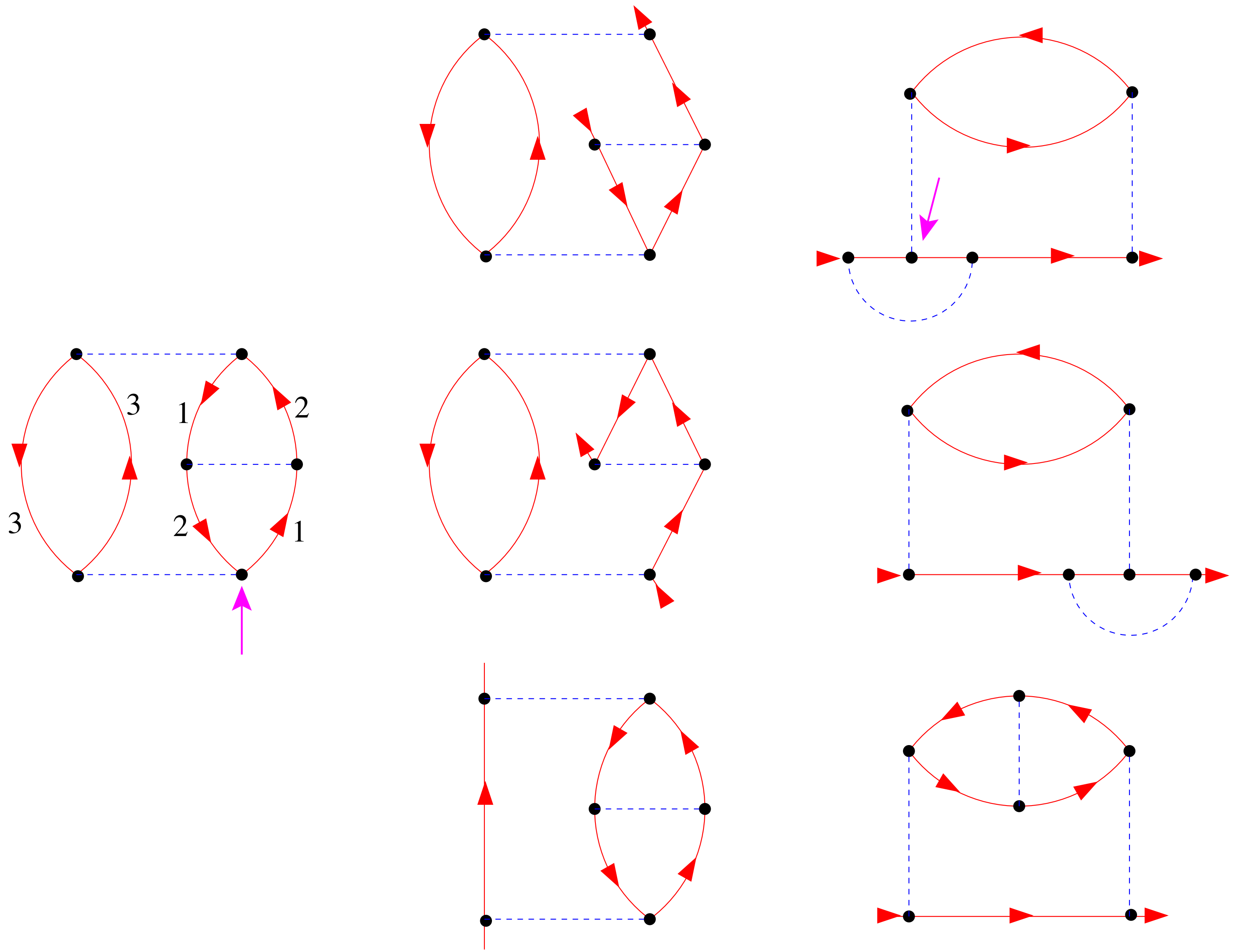
Example, cont'd



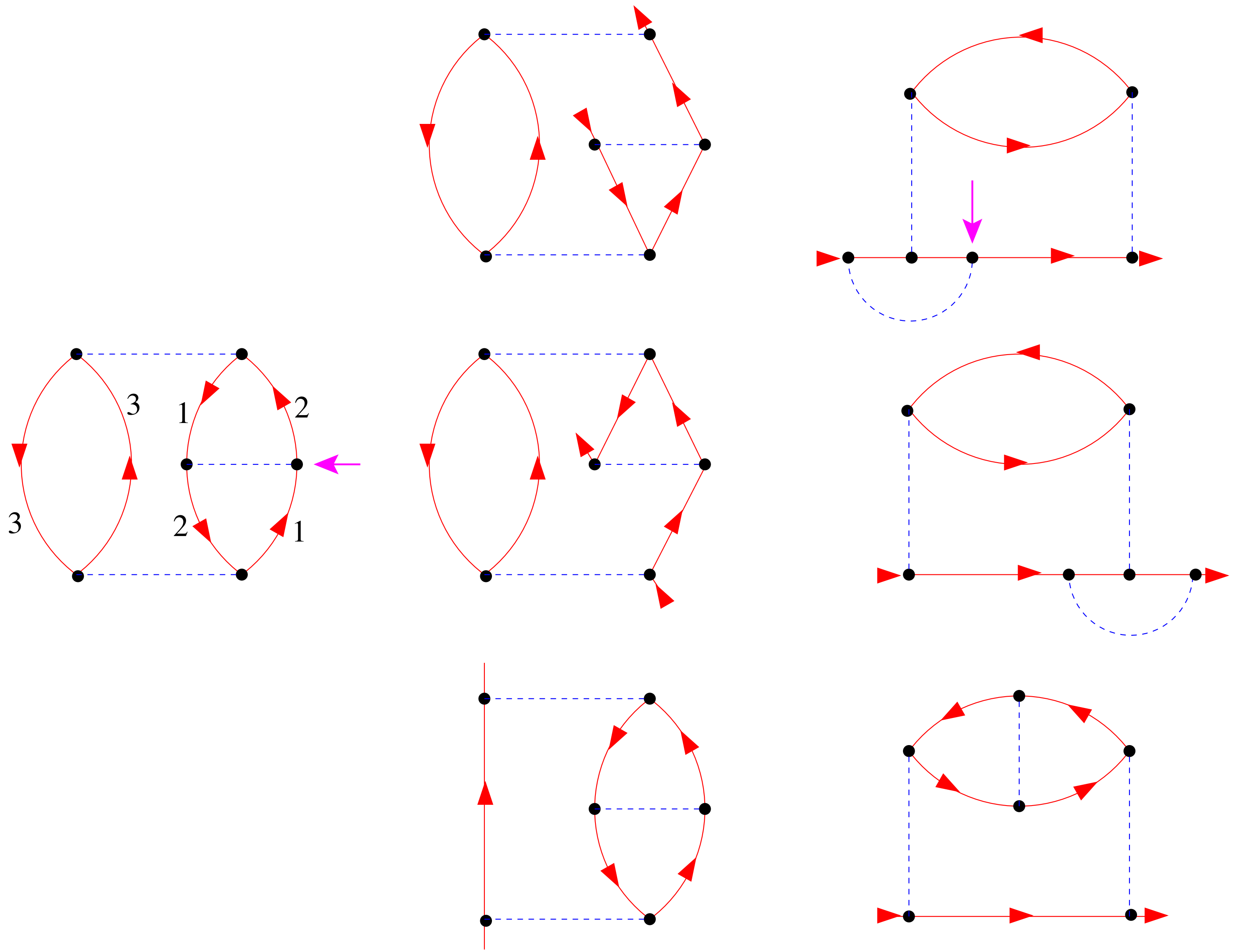
Example, cont'd



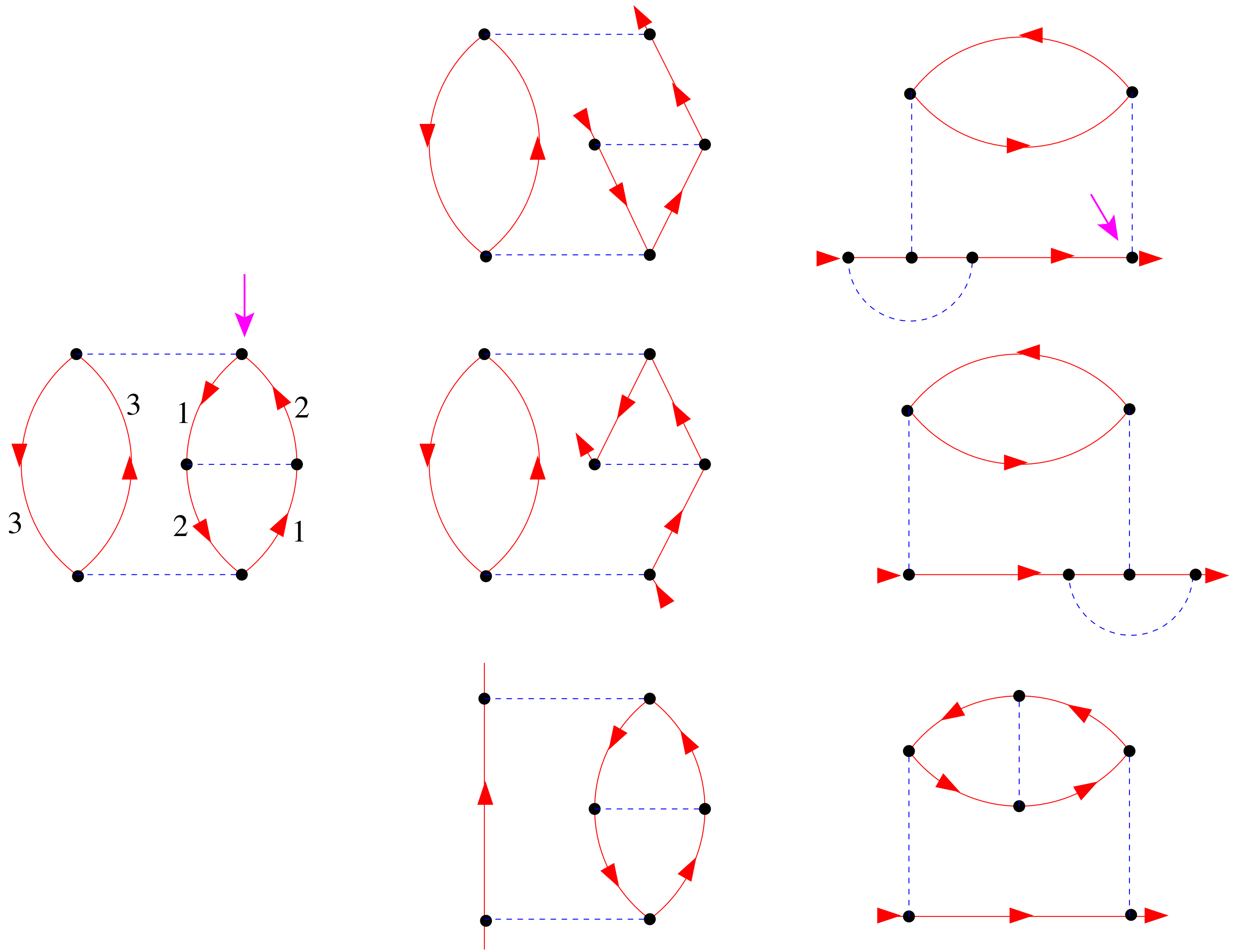
Example, cont'd



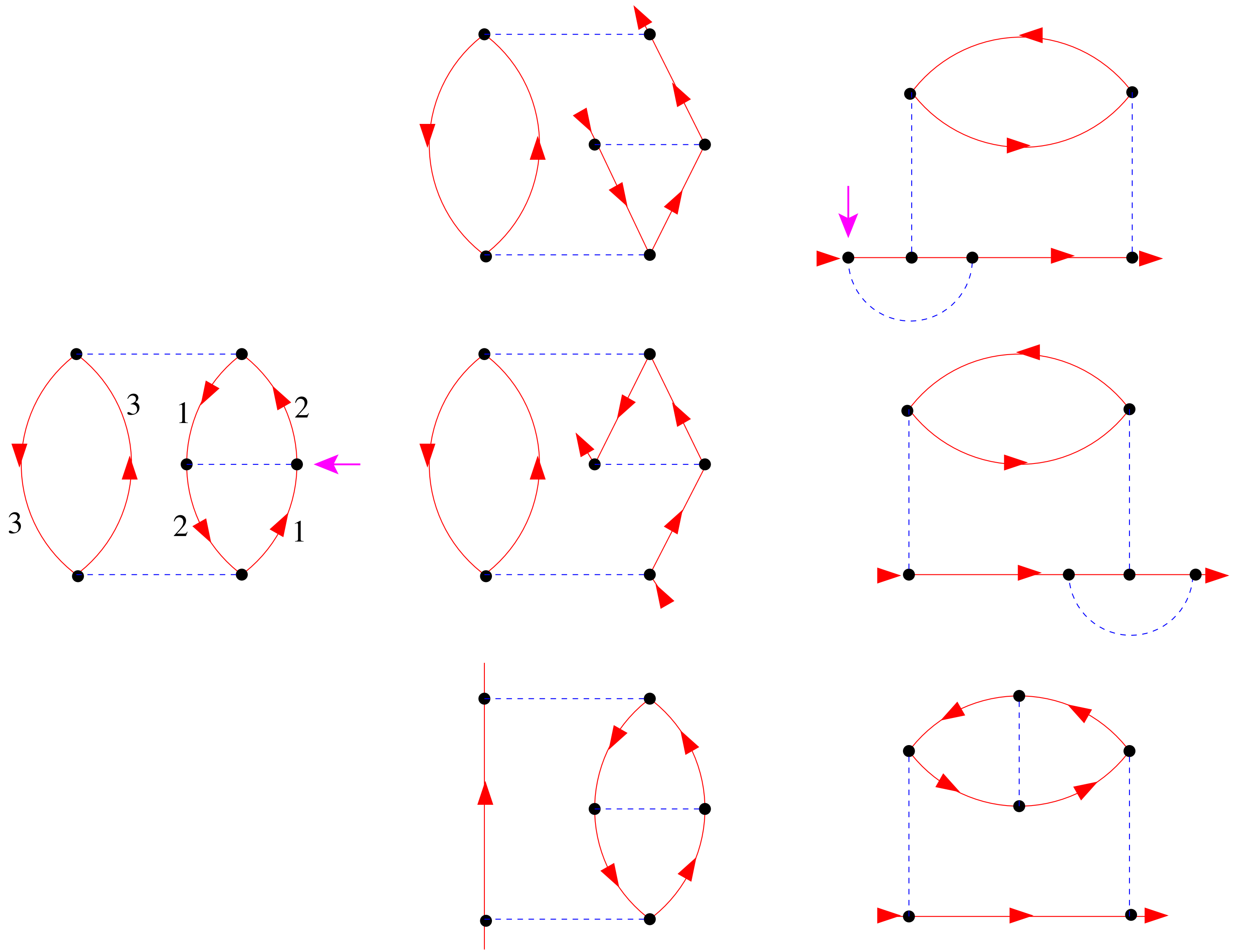
Example, cont'd



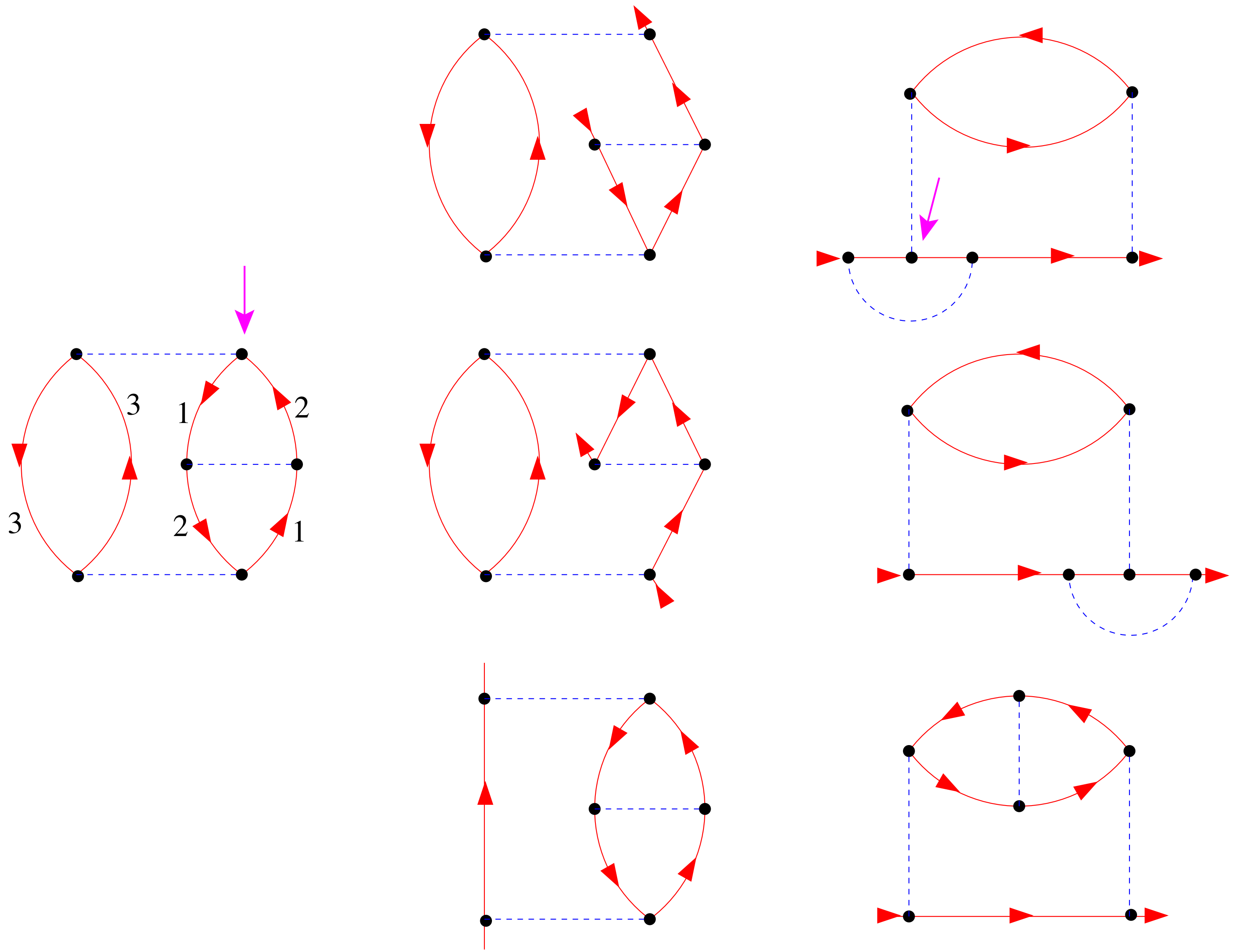
Example, cont'd



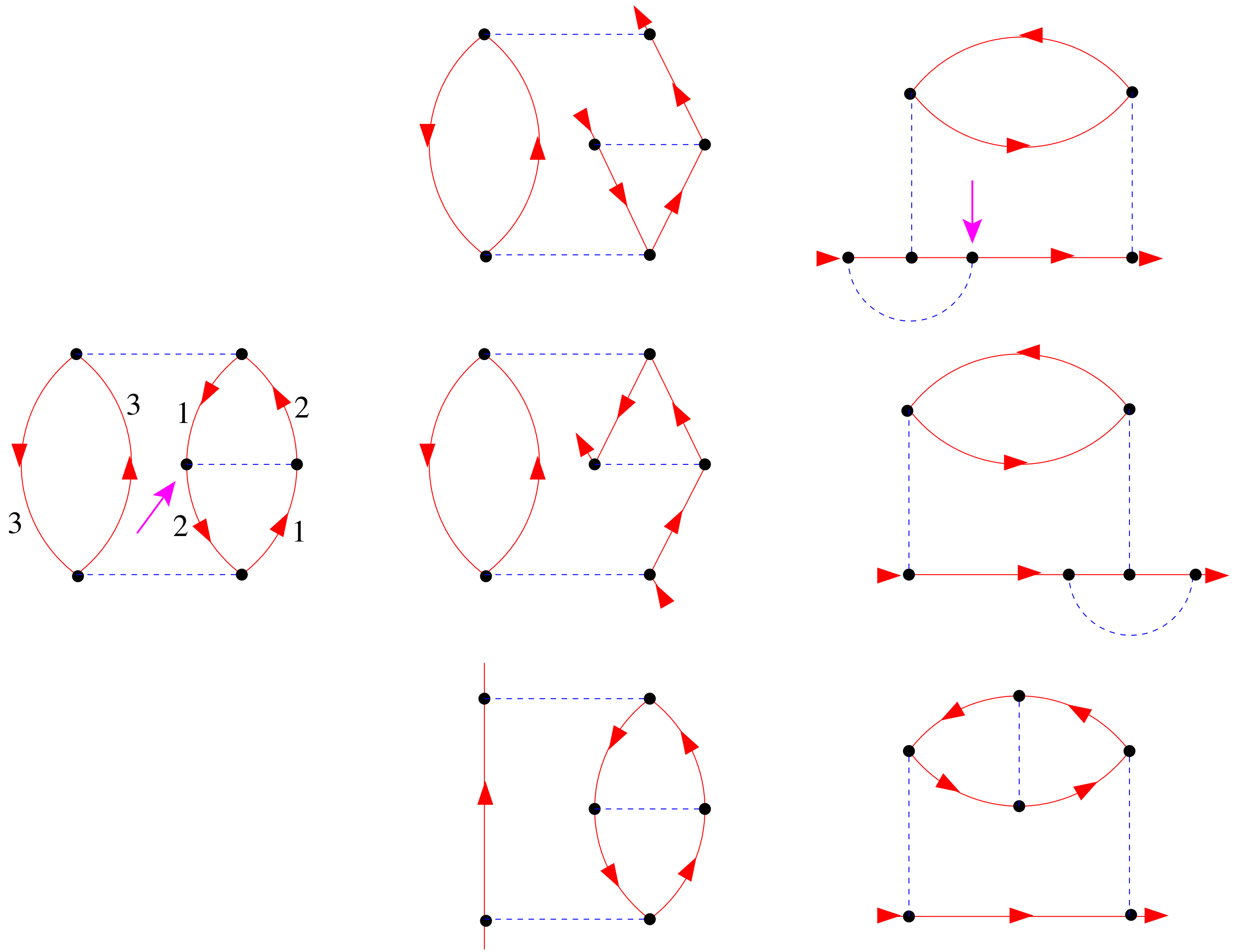
Example, cont'd



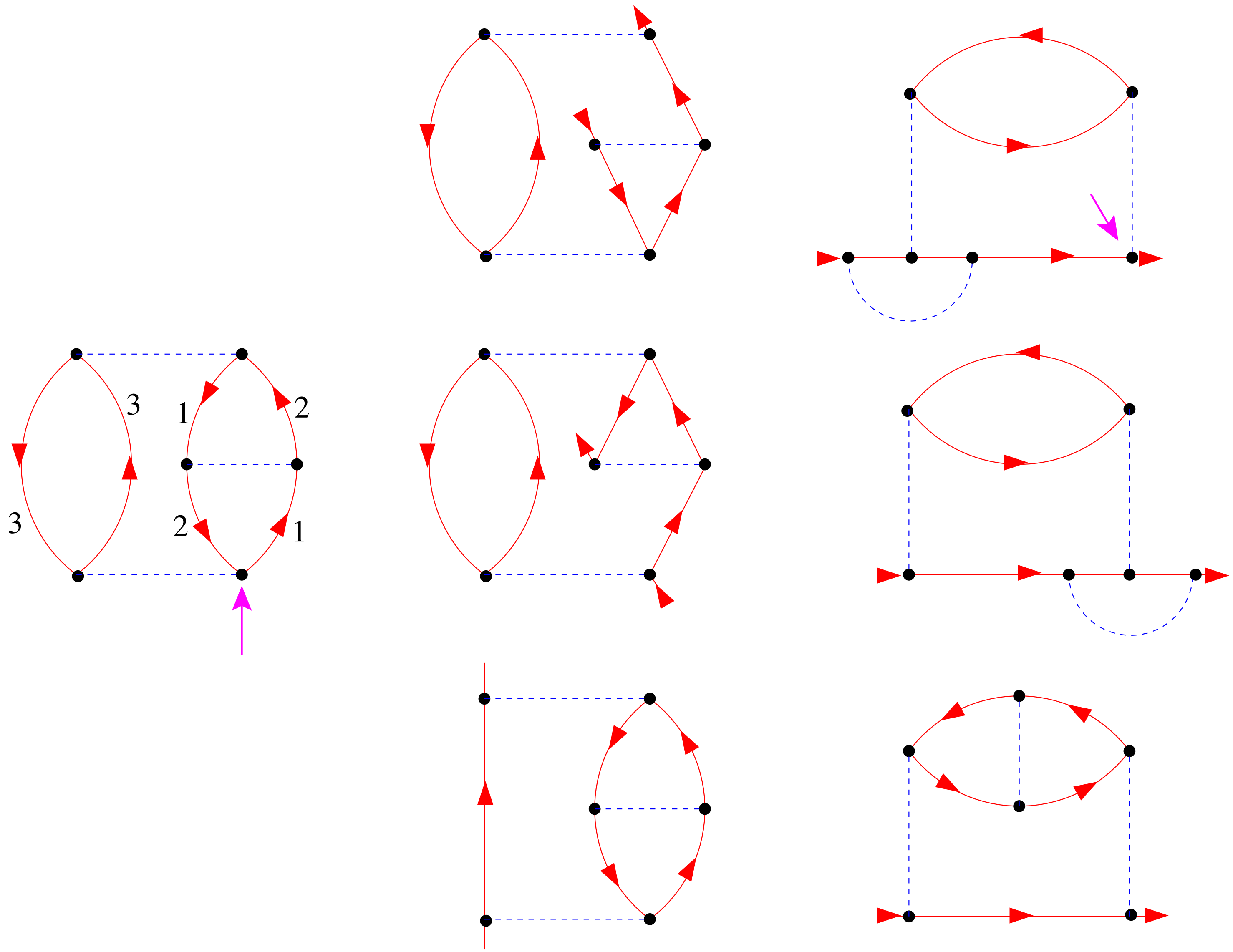
Example, cont'd



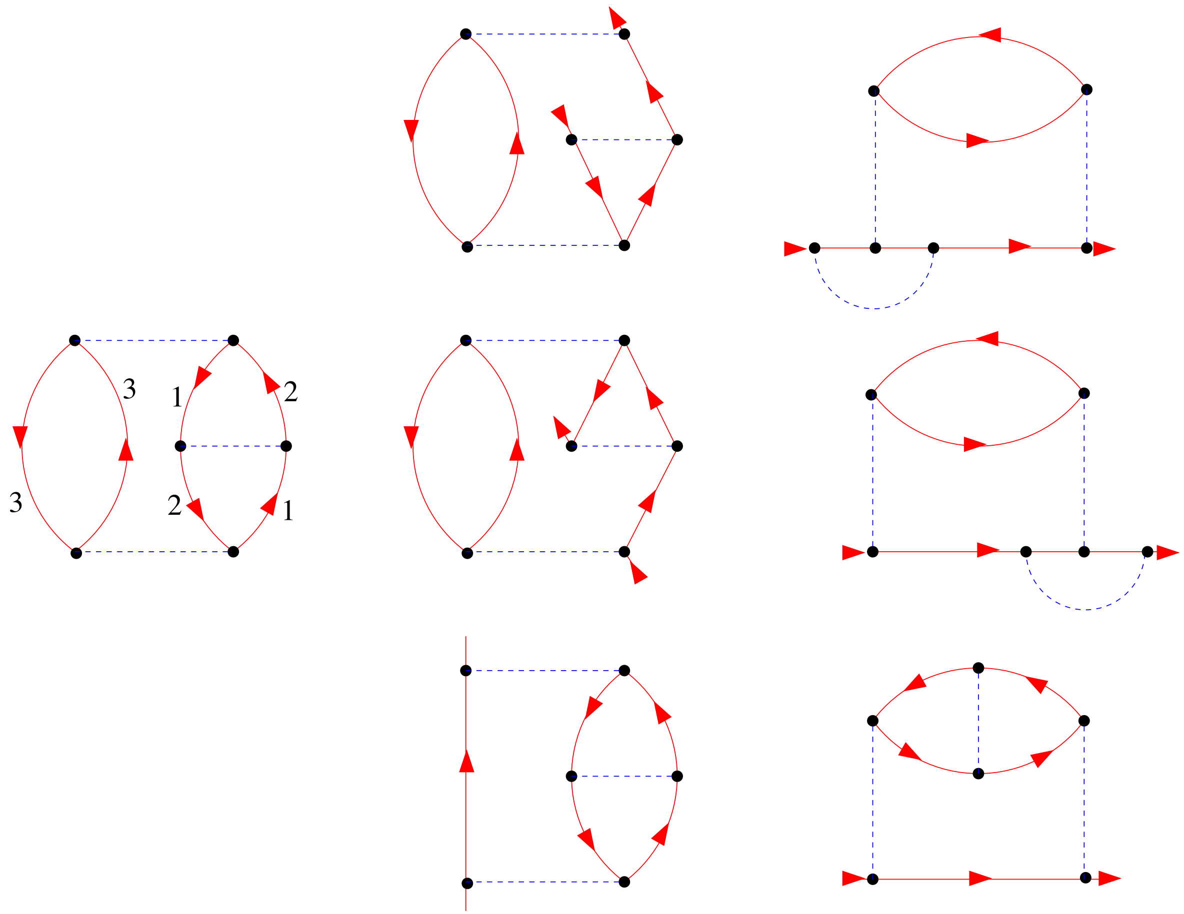
Example, cont'd



Example, cont'd



Example, cont'd



- The diagram has $n = 3$ and $S = 2 \rightarrow 3$ classes with 2 members each
- By successively opening the lines we get 3 different self-energy diagrams
- Each of them is produced 2 times

We have seen that the derivative

$$\frac{\partial \Phi[\mathbf{G}]}{\partial G_{\alpha,\beta}(\mathbf{k}, i\omega_\nu)}$$

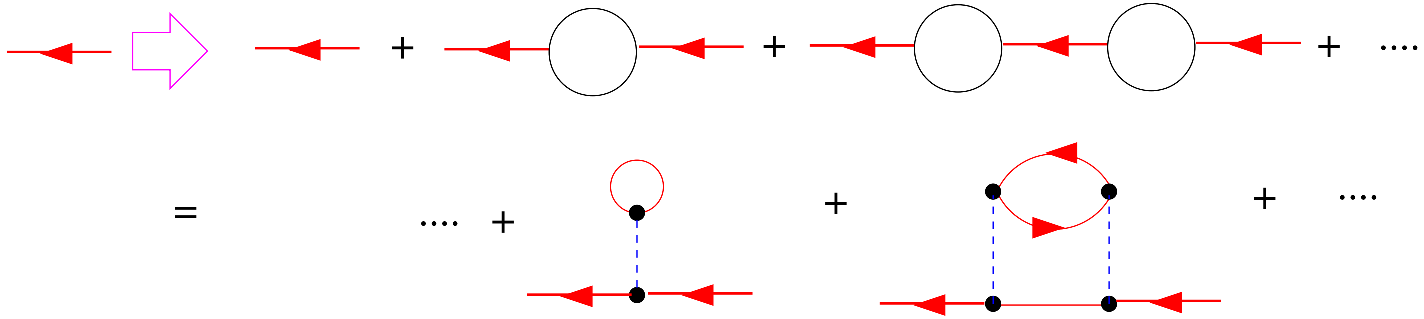
gives precisely all skeleton diagrams for $\Sigma_{\beta,\alpha}(\mathbf{k}, i\omega_\nu)$ but with the the Green's function $\mathbf{G}$ used for all Green's function lines (and a prefactor $1/\beta$)

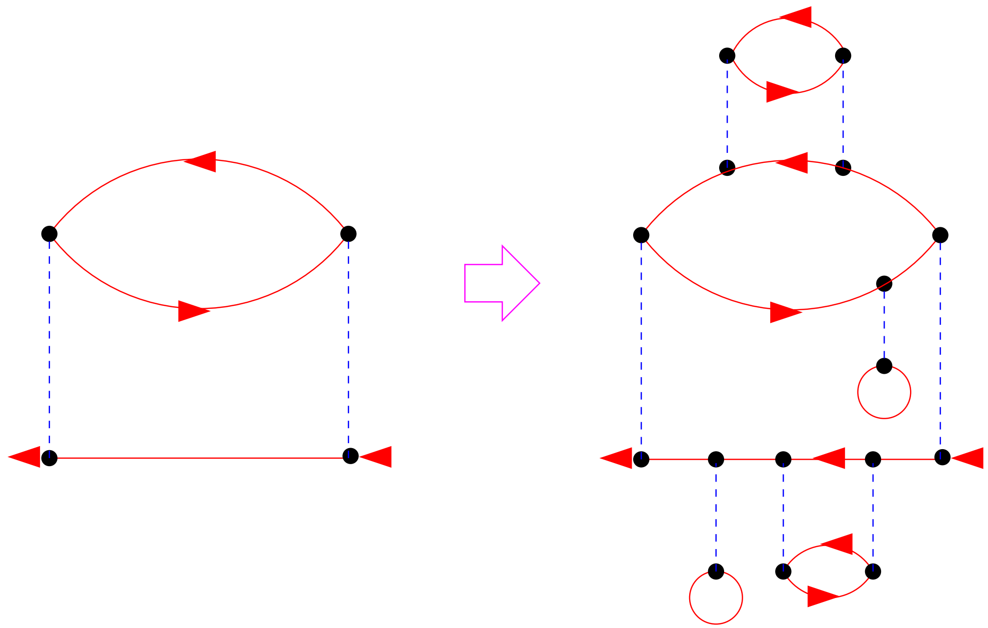
If $\mathbf{G}$ is the exact Green's function this is the exact self-energy

Therefore: If $\mathbf{G}$ is the exact Green's function we have

$$\frac{\partial \Phi[\mathbf{G}]}{\partial G_{\alpha,\beta}(\mathbf{k}, i\omega_\nu)} = \frac{1}{\beta}\,\Sigma_{\beta,\alpha}(\mathbf{k}, i\omega_\nu)$$

This also goes the other way round





By drawing all skeleton-diagrams for the self-energy and ‘translating’ Green’s function lines into the full Green’s function instead of the noninteracting one the total self-energy is obtained

We have seen that the derivative

$$\frac{\partial \Phi[\mathbf{G}]}{\partial G_{\alpha,\beta}(\mathbf{k}, i\omega_\nu)}$$

gives precisely all skeleton diagrams for $\Sigma_{\beta,\alpha}(\mathbf{k}, i\omega_\nu)$ but with the the Green's function $\mathbf{G}$ used for all Green's function lines (and a prefactor $1/\beta$)

If $\mathbf{G}$ is the exact Green's function this is the exact self-energy

Therefore: If $\mathbf{G}$ is the exact Green's function we have

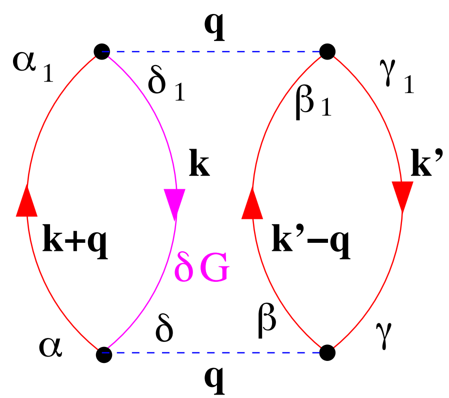
$$\frac{\partial \Phi[\mathbf{G}]}{\partial G_{\alpha,\beta}(\mathbf{k}, i\omega_\nu)} = \frac{1}{\beta}\, \Sigma_{\beta,\alpha}(\mathbf{k}, i\omega_\nu)$$

We saw that $\boldsymbol{\Sigma}(\boldsymbol{k}, \omega)$ can be obtained from $\Phi[\boldsymbol{G}]$ by 'opening' Green's function lines

The question is then: can this be reversed, that means:

Can $\Phi[\boldsymbol{G}]$ be obtained from $\boldsymbol{\Sigma}(\boldsymbol{k}, \omega)$ by 'reconnecting' the two entry points by a Green's function?

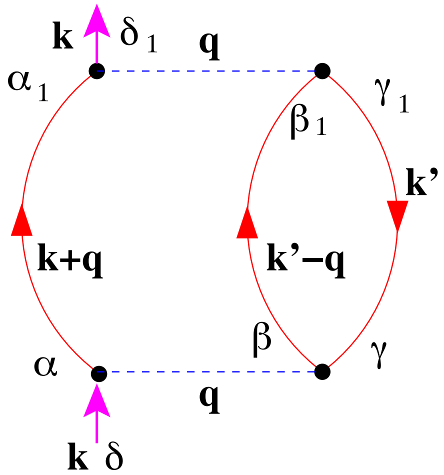
Factoring out the variation δG 'fixes' the momentum, frequency and band indices of the remaining diagram



$$\left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma,\delta} \sum_{\alpha_1,\beta_1,\gamma_1,\delta_1} \sum_{\nu,\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{q},-\mathbf{q})$$

$$G_{\alpha_1,\alpha}(\mathbf{k}+\mathbf{q}, i\omega_\nu + \omega_\mu)\ \delta G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu)\ G_{\beta_1,\beta}(\mathbf{k}'-\mathbf{q}, i\omega_{\nu'} - i\omega_\mu)\ G_{\gamma,\gamma_1}(\mathbf{k}', i\omega_{\nu'})$$

Factoring out the variation δG 'fixes' the momentum, frequency and band indices of the remaining diagram



$$\delta G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu) \left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma} \sum_{\alpha_1,\beta_1,\gamma_1} \sum_{\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k}, \mathbf{k}', \mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q}, \mathbf{k}'-\mathbf{q}, -\mathbf{q})$$

$$G_{\alpha_1,\alpha}(\mathbf{k}+\mathbf{q}, i\omega_\nu + \omega_\mu) \qquad G_{\beta_1,\beta}(\mathbf{k}'-\mathbf{q}, i\omega_{\nu'} - i\omega_\mu)\, G_{\gamma,\gamma_1}(\mathbf{k}', i\omega_{\nu'})$$

The correct operation to 'undo' the opening of a line therefore is something like

$$\Phi^{(n)}[\mathbf{G}] \;\propto\; \frac{1}{\beta} \sum_{\nu,\mathbf{k}} \sum_{\alpha,\beta} \mathbf{G}_{\alpha,\beta}(\mathbf{k}, i\omega_\nu) \mathbf{\Sigma}^{(s,n)}_{\beta,\alpha}(\mathbf{k}, i\omega_\nu)$$

$$= \frac{1}{\beta} \sum_{\nu,\mathbf{k}} \text{trace } \mathbf{G}(\mathbf{k}, i\omega_\nu)\ \mathbf{\Sigma}^{(s,n)}(\mathbf{k}, i\omega_\nu)$$

$\Phi^{(n)}$ is the sum of all n^{th} order diagrams for Φ: closed, linked skeleton diagrams, with Green's function lines standing for the full Green's function $\mathbf{G}$

$\mathbf{\Sigma}^{(s,n)}_{\beta,\alpha}(\mathbf{k}, i\omega_\nu)$ is the sum of all n^{th} order skeleton diagrams for the self-energy with Green's function lines standing for the full Green's function $\mathbf{G}$

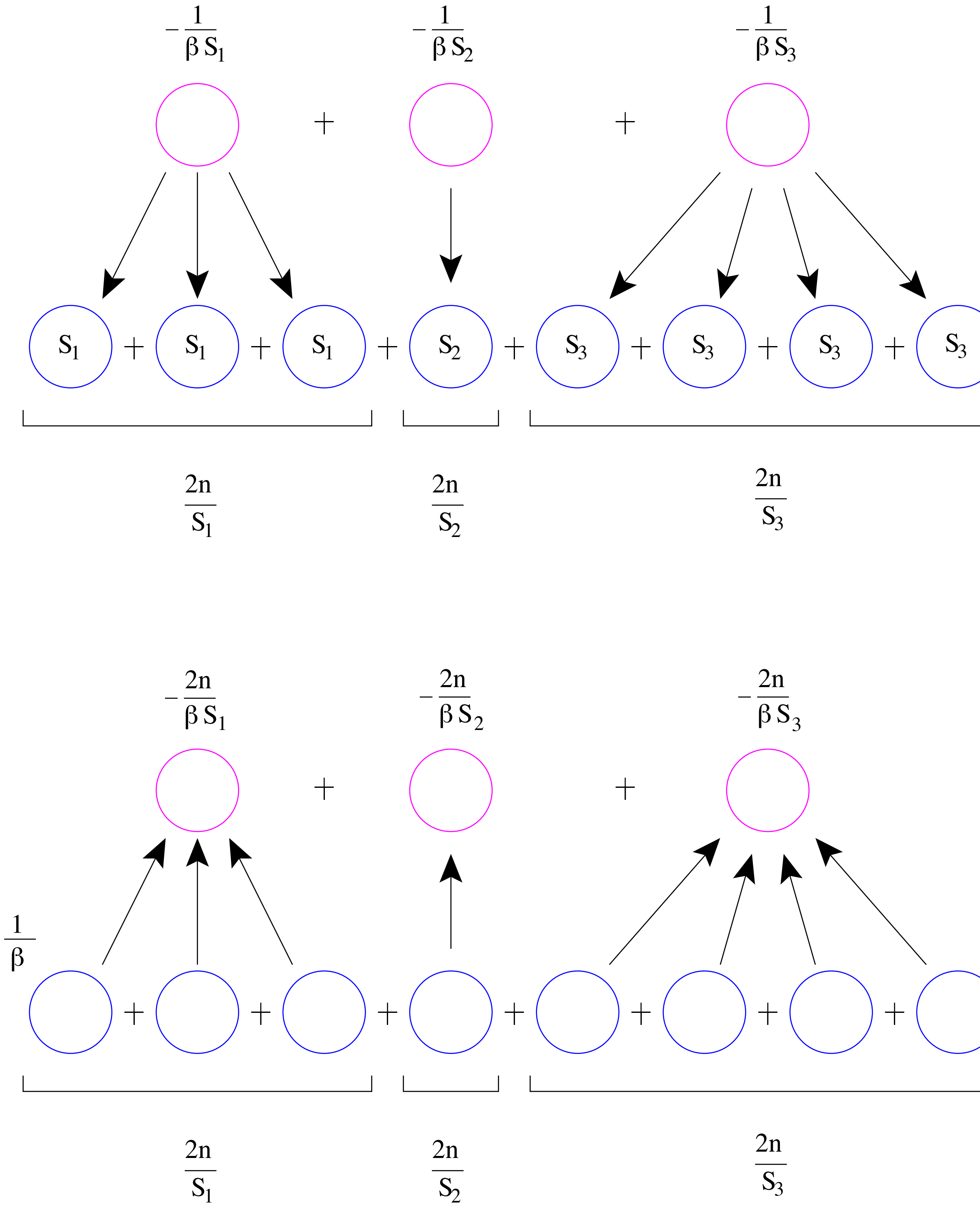
We include only skeleton-diagrams for $\mathbf{\Sigma}$ because we only want skeleton diagrams for Φ

However, again we need to be careful about prefactors!

We consider n^{th}-order diagrams for Φ and Σ

This shows

$$\Phi^{(n)} = \frac{1}{2n\beta} \sum_{\nu,\mathbf{k}} \text{trace } \mathbf{G}(\mathbf{k}, i\omega_\nu) \, \mathbf{\Sigma}^{(s,n)}(\mathbf{k}, i\omega_\nu)$$



Summary of the properties of the Luttinger-Ward functional

- The Luttinger Ward functional involves only the interaction matrix elements $V_{\alpha\beta\gamma\delta}$ of the Hamiltonian, but not the single particle matrix elements $t_{\alpha\beta}$
- The Luttinger-Ward functional is the generating functional of the self-energy, which is obtained by opening Green's function lines

$$\frac{\partial\Phi}{\partial G_{\alpha,\beta}(\mathbf{k}, i\omega_\nu)} = \frac{1}{\beta}\, \Sigma_{\beta,\alpha}(\mathbf{k}, i\omega_\nu)$$

- The Luttinger-Ward functional can also be written by 'closing' the open ends in the self-energ - however, there is an extra factor of $1/2n$ (n is the order of the self-energy diagram) which makes resummation impossible

$$\begin{aligned}\Phi &= \sum_n \Phi^{(n)} \\ &= \frac{1}{\beta} \sum_n \frac{1}{2n} \sum_{\nu,\mathbf{k}} \text{trace } \mathbf{G}(\mathbf{k}, i\omega_\nu)\, \mathbf{\Sigma}^{(s,n)}(\mathbf{k}, i\omega_\nu)\end{aligned}$$

$\mathbf{\Sigma}^{(s,n)}$ is the n^{th} order 'skeleton self-energy'

We now want to proove that $\Omega' = \Omega$ thereby following the original proof by Luttinger and Ward:

- We replace $H \to H_0 + \lambda H_1$
- We show $\Omega' = \Omega$ for $\lambda = 0$ (the case of noninteracting electrons)
- We calculate $\lambda \partial_\lambda \, \Omega$
- We calculate $\lambda \partial_\lambda \, \Omega'$ and show that it is equal to $\lambda \partial_\lambda \, \Omega$

Obviously this prooves the equality of Ω' and Ω

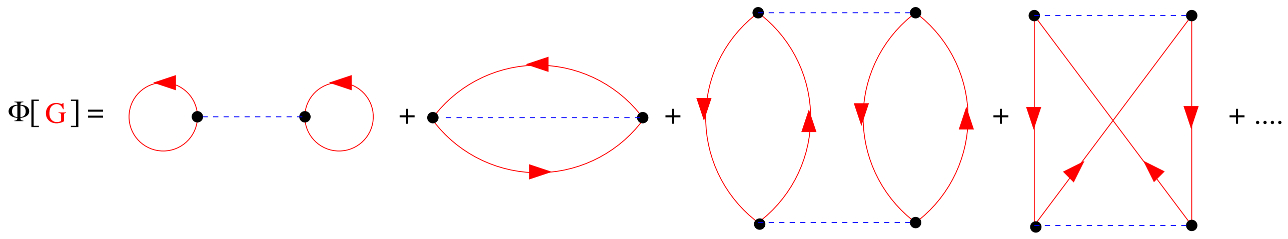
Calculation of $\lambda \, \frac{\partial \Omega'}{\partial \lambda}$

$$\Omega' = -\lim_{\eta \to 0^+} \frac{1}{\beta} \sum_{\mathbf{k},\nu} e^{i\omega_\nu \eta} \left[\ln \, \det \left(-\mathbf{G}^{-1}(\mathbf{k}, i\omega_\nu) \right) + \text{trace} \left(\mathbf{G}(\mathbf{k}, i\omega_\nu) \, \mathbf{\Sigma}(\mathbf{k}, i\omega_\nu) \right) \right] + \Phi \, [\mathbf{G}].$$

Reminder: we replaced $H \to H_0 + \lambda H_1$ - a variation $\lambda \to \lambda + \delta\lambda$ has two different effects

- The self-energy $\mathbf{\Sigma}$ will change
- The interaction lines in the Luttinger-Ward functional will change

  (since $H_1 \to \lambda \, H_1$ they carry a factor of λ!)



We treat these two variations separately and first consider the variation of Ω' under a change $\mathbf{\Sigma} \to \mathbf{\Sigma} + \delta\mathbf{\Sigma}$

Calculation of $\frac{\partial \Omega'}{\partial \Sigma}$

To avoid calculations with many indices we treat only the case of a single spinless band

(see the notes for the full multi-band case)

$$\Omega' = -\lim_{\eta \to 0^+} \frac{1}{\beta} \sum_{\mathbf{k},\nu} e^{i\omega_\nu \eta} \left[\ln \, \text{det} \left(-\mathbf{G}^{-1}(\mathbf{k}, i\omega_\nu) \right) + \text{trace} \left(\mathbf{G}(\mathbf{k}, i\omega_\nu) \, \mathbf{\Sigma}(\mathbf{k}, i\omega_\nu) \right) \right] + \Phi \left[\mathbf{G} \right]$$

then becomes

$$\Omega' = -\lim_{\eta \to 0^+} \frac{1}{\beta} \sum_{\mathbf{k},\nu} e^{i\omega_\nu \eta} \left[\ln \left(-G^{-1}(\mathbf{k}, i\omega_\nu) \right) + G(\mathbf{k}, i\omega_\nu) \, \Sigma(\mathbf{k}, i\omega_\nu) \right] + \Phi \left[G \right]$$

- We need to differentiate this with respect to $\Sigma(\mathbf{k}, i\omega_\nu)$
- The first two terms are a sum over terms with different $\mathbf{k}$ and $i\omega_\nu$ - only one term contributes
- All G and Σ in this term have the same argument $(\mathbf{k}, i\omega_\nu)$ - we omit this for simlicity

$$\Omega' = -\lim_{\eta\to 0^+}\frac{1}{\beta}\sum_{\mathbf{k},\nu} e^{i\omega_\nu\eta}\left[\ln\left(-G^{-1}(\mathbf{k},i\omega_\nu)\right) + G(\mathbf{k},i\omega_\nu)\,\Sigma(\mathbf{k},i\omega_\nu)\right] + \Phi\,[G]$$

Then we have

$$\frac{\partial\Omega'}{\partial\Sigma} = -\frac{1}{\beta}\left[\frac{1}{(-G^{-1})}\,\frac{\partial(-G^{-1})}{\partial\Sigma} + \frac{\partial G}{\partial\Sigma}\,\Sigma + G\right] + \frac{\partial\Phi}{\partial G(\mathbf{k},i\omega_\nu)}\,\frac{\partial G(\mathbf{k},i\omega_\nu)}{\partial\Sigma(\mathbf{k},i\omega_\nu)}$$

Now we use the Dyson equation

$$-G^{-1}(\mathbf{k},i\omega_\nu) = -i\omega_\nu + \frac{1}{\hbar}(E(\mathbf{k})-\mu) + \Sigma(\mathbf{k},i\omega_\nu)$$

$$\to \frac{\partial(-G^{-1})}{\partial\Sigma} = 1$$

So that

$$\frac{\partial\Omega'}{\partial\Sigma} = -\frac{1}{\beta}\left[-G + \frac{\partial G}{\partial\Sigma}\,\Sigma + G\right] + \frac{\partial\Phi}{\partial G(\mathbf{k},i\omega_\nu)}\,\frac{\partial G(\mathbf{k},i\omega_\nu)}{\partial\Sigma(\mathbf{k},i\omega_\nu)}$$

We had

$$\frac{\partial \Omega'}{\partial \Sigma} = -\frac{1}{\beta}\frac{\partial G}{\partial \Sigma}\Sigma + \frac{\partial \Phi}{\partial G(\mathbf{k}, i\omega_\nu)}\frac{\partial G(\mathbf{k}, i\omega_\nu)}{\partial \Sigma(\mathbf{k}, i\omega_\nu)}$$

Now we use the fact that Φ is the generating functional of Σ

$$\frac{\partial \Phi}{\partial G(\mathbf{k}, i\omega_\nu)} = \frac{1}{\beta}\Sigma(\mathbf{k}, i\omega_\nu)$$

Then we have

$$\frac{\partial \Omega'}{\partial \Sigma} = -\frac{1}{\beta}\frac{\partial G}{\partial \Sigma}\Sigma + \frac{1}{\beta}\Sigma\;\frac{\partial G}{\partial \Sigma} = 0$$

Ω' is stationary under variations of the self-energy

Once we have shown that $\Omega' = \Omega$ this prooves a variational principle of central importance: The Grand Canonical Potential of an interacting Fermi system is stationary with respect to variations of its self-energy

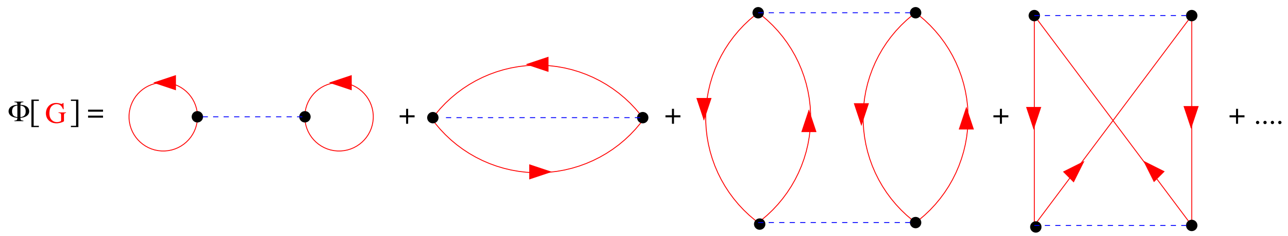
Calculation of $\lambda \frac{\partial \Omega'}{\partial \lambda}$

$$\Omega' = -\lim_{\eta \to 0^+} \frac{1}{\beta} \sum_{\mathbf{k},\nu} e^{i\omega_\nu \eta} \left[\ln \ \text{det} \left(-\mathbf{G}^{-1}(\mathbf{k}, i\omega_\nu) \ \right) + \text{trace} \left(\mathbf{G}(\mathbf{k}, i\omega_\nu) \ \mathbf{\Sigma}(\mathbf{k}, i\omega_\nu) \right) \ \right] + \Phi \ [\mathbf{G}].$$

Reminder: we replaced $H \to H_0 + \lambda H_1$ - a variation $\lambda \to \lambda + \delta\lambda$ has two different effects

- The self-energy $\mathbf{\Sigma}$ will change - but the corresponding first order change of Ω' is zero!
- The interaction lines in the Luttinger-Ward functional will change

  (since $H_1 \to \lambda \ H_1$ they carry a factor of λ!)



Accordingly we study the change of Φ under a change of λ (prefactor of all interaction lines) when Σ is kept fixed

This is in fact a rather simple calculation: we again split the Luttinger-Ward functional

$$\Phi = \sum_n \Phi^{(n)}$$

whereby $\Phi^{(n)}$ is the sum of diagrams with n interaction lines - which is proportional to λ^n

But:

$$\lambda \frac{\partial \lambda^n}{\partial \lambda} = n\lambda^n$$

It follows that ($\mathbf{\Sigma}^{(s,n)}$ denotes all n^{th} order self-energy skeleton diagrams)

$$\begin{aligned}
\lambda\frac{d\Omega'}{d\lambda} = \lambda\frac{d\Phi}{d\lambda} &= \sum_n n \, \Phi^{(n)} \\
&= \sum_n n \, \frac{1}{2\beta n} \sum_{\nu,\mathbf{k}} \text{trace } \mathbf{G}_\lambda(\mathbf{k}, i\omega_\nu)\mathbf{\Sigma}_\lambda^{(s,n)}(\mathbf{k}, i\omega_\nu) \\
&= \frac{1}{2\beta} \sum_{\nu,\mathbf{k}} \text{trace } \mathbf{G}_\lambda(\mathbf{k}, i\omega_\nu) \left(\sum_n \mathbf{\Sigma}_\lambda^{(s,n)}(\mathbf{k}, i\omega_\nu) \right) \\
&= \frac{1}{2\beta} \sum_{\nu,\mathbf{k}} \text{trace } \mathbf{G}_\lambda(\mathbf{k}, i\omega_\nu) \, \mathbf{\Sigma}_\lambda(\mathbf{k}, i\omega_\nu) = \lambda\frac{d\Omega}{d\lambda}
\end{aligned}$$

This is precisely the same result we obtained for $\lambda\partial_\lambda \, \Omega$!

Summary of the Proof

- The Grand Canonical Potential of an interacting Fermi system is given by

$$\Omega \;=\; -\lim_{\eta\to 0^+}\frac{1}{\beta}\sum_{\mathbf{k},\nu} e^{i\omega_\nu\eta}\;\Big[\ln\;\mathrm{det}\left(-\mathbf{G}^{-1}(\mathbf{k},i\omega_\nu)\;\right)+\mathrm{trace}\left(\mathbf{G}(\mathbf{k},i\omega_\nu)\;\boldsymbol{\Sigma}(\mathbf{k},i\omega_\nu)\right)\;\Big]+\Phi\;[\mathbf{G}]$$

- Ω is stationary with respect to variations of the self-energy

$$\frac{\partial\Omega}{\partial\Sigma_{\alpha\beta}(\mathbf{k},i\omega_\nu)}=0$$

- The Luttinger-Ward functional is the generating functional of the self-energy

$$\frac{\partial\Phi}{\partial G_{\alpha,\beta}(\mathbf{k},i\omega_\nu)}=\frac{1}{\beta}\,\Sigma_{\beta,\alpha}(\mathbf{k},i\omega_\nu)$$

Applications of the Luttinger-Ward functional: Conserving Approximations

- We consider a translationally invariant system $V(\mathbf{r}) = 0$ - the Hamiltonian is

$$H = \frac{\hbar^2}{2m} \int d\mathbf{r}\ \nabla \Psi^\dagger(\mathbf{r}) \cdot \nabla \Psi(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}'\ \Psi^\dagger(\mathbf{r}) \Psi^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \Psi(\mathbf{r}') \Psi(\mathbf{r}).$$

- We assume that a time-dependent perturbation $H_p = \int d\mathbf{r}\ U(\mathbf{r}, t)\ n(\mathbf{r})$
- Then the change of the expectation value of any operator $\hat{A}(\mathbf{r})$ is

$$\delta \langle \hat{A}(\mathbf{r}) \rangle (t) = \frac{1}{\hbar} \int d\mathbf{r}' \int_{-\infty}^{\infty} dt'\ G^R_{A,n}(\mathbf{r}t, \mathbf{r}'t')\ U\ (\mathbf{r}', t')$$

- We may choose $\hat{A}$ to be electron density or electron current - we obtain the density $\delta n(\mathbf{r}, t)$ and current $\mathbf{j}(\mathbf{r}, t)$
- However, density and current must obey conservation laws

$$\begin{aligned} \frac{\partial \delta n(\mathbf{r})}{\partial t} + \nabla \cdot \delta \mathbf{j}(\mathbf{r}) &= 0, \\ \frac{d}{dt} \int d\mathbf{r}\ m \delta \mathbf{j}(\mathbf{r}) &= \int d\mathbf{r}\, (-\nabla U(\mathbf{r}, t))\, n(\mathbf{r}, t) \\ \frac{d}{dt} \langle H \rangle &= \int d\mathbf{r}\, (-\nabla U(\mathbf{r}, t)) \cdot \delta \mathbf{j}(\mathbf{r}) \end{aligned}$$

For the *exact* $\delta n(\mathbf{r},t)$ and $\mathbf{j}(\mathbf{r},t)$ the conservation laws of course are obeyed - but in general we have to make some approximation to calculate the retarded Green's function in

$$\delta \,\langle \hat{A}(\mathbf{r})\rangle(t) \;=\; \frac{1}{\hbar}\int d\mathbf{r}' \int_{-\infty}^{\infty} dt'\; G^R_{A,n}(\mathbf{r}t,\mathbf{r}'t')\; U\;(\mathbf{r}',t')$$

The question is: can we find approximations to $G^R_{A,n}(\mathbf{r}t,\mathbf{r}'t')$ such that the resulting approximate $\delta n(\mathbf{r},t)$ and $\mathbf{j}(\mathbf{r},t)$ obey the conservation laws?

This question was addressed in the famous papers by Kadanoff and Baym

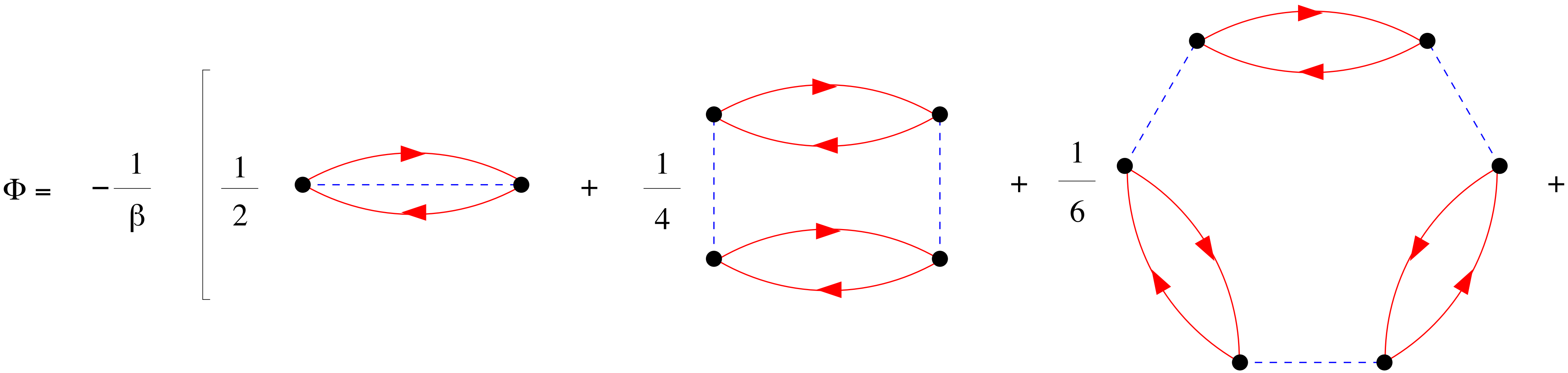
Their answer: if we construct an approximate Luttinger-Ward functional $\tilde{\Phi}[\mathbf{G}]$ by retaining only a subclass of skeleton diagrams and defining

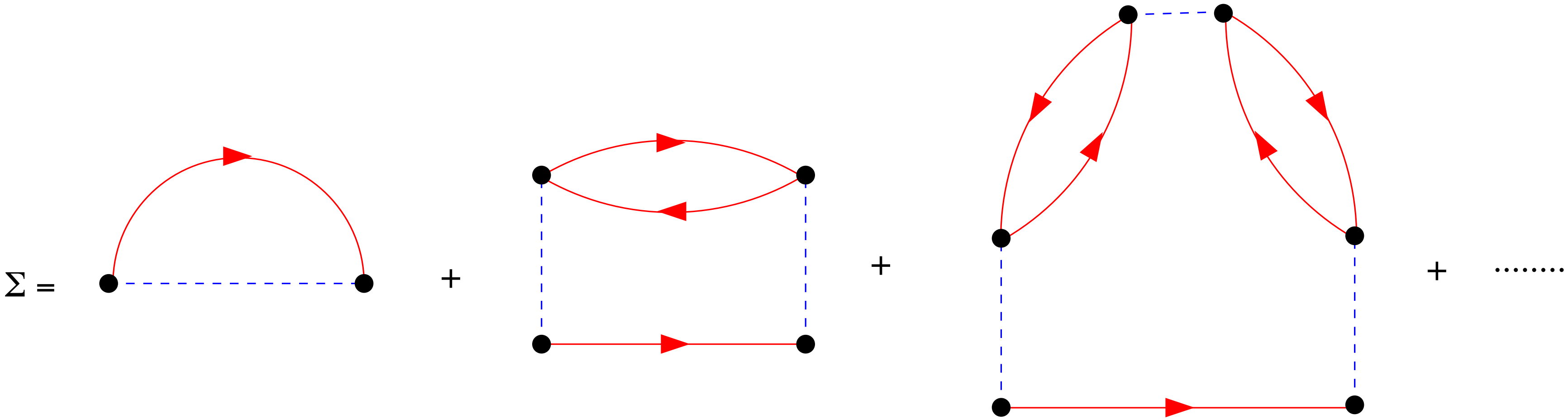
$$-\frac{1}{\beta}\tilde{\Sigma}_{\alpha,\beta}(\mathbf{k},i\omega_\nu) \;=\; \frac{\partial\tilde{\Phi}[\mathbf{G}]}{\partial G_{\beta,\alpha}(\mathbf{k},i\omega_\nu)} \Rightarrow \tilde{\Sigma} = \tilde{\Sigma}[G] \Rightarrow G^{-1} = G_0^{-1} - \tilde{\Sigma}[G]$$

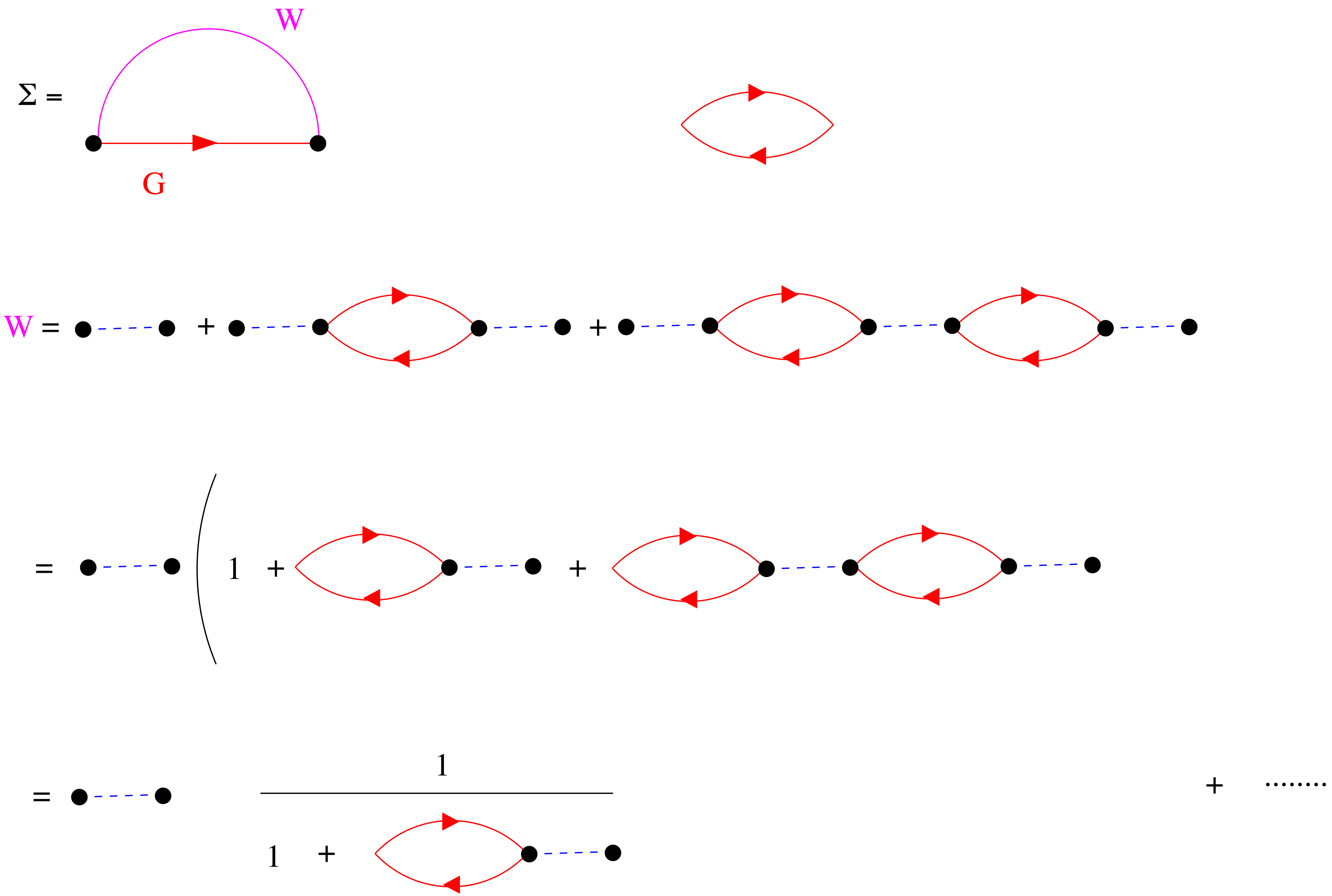
the resulting theory does obey the conservation laws

This is difficult to proove - in the notes the proof is given for the continuity equation.....

A famous example for such a conserving approximation is the GW-approximation







Σ =
W
G
W =
+
+
=
1
+
+
=
1
1
+
+ ....

Summary

- The Grand Canonical Potential of an interacting Fermi system can be expressed as a functional of its Green's function
- This involves the Luttinger-Ward functional which is defined as a sum over infinitely many Feynman diagrams
- The expression for Ω is the starting point for important results such as the Luttinger theorem
- The Luttinger-Ward functional is the generating functional for the self-energy and is of considerable importance for obtaining conserving approximations
- Ω is stationary with respect to variations of the self-energy and this can be used to derive many schemes to compute the self-energy

Calculation of $\langle \lambda H_1 \rangle_\lambda$

This can be obtained from the Green's function

$$G_{\alpha,\beta}(\tau) \;=\; -\Theta(\tau)\,\langle\, c_\alpha(\tau)\, c_\beta^\dagger \,\rangle_{th} + \Theta(-\tau)\,\langle\, c_\beta^\dagger\, c_\alpha(\tau)\,\rangle_{th}$$

We assume $\tau < 0$ and set $\beta = \alpha$

$$\begin{aligned} G_{\alpha,\alpha}(\tau) &= \langle c_\alpha^\dagger \;\; c_\alpha(\tau)\rangle_{th} \\ &= \langle c_\alpha^\dagger \;\; e^{\frac{\tau}{\hbar}K}\; c_\alpha\; e^{-\frac{\tau}{\hbar}K}\;\rangle_{th} \\ \Rightarrow -\hbar\,\frac{\partial G_{\alpha,\alpha}(\tau)}{\partial\tau} &= \langle c_\alpha^\dagger \;\; e^{\frac{\tau}{\hbar}K}\;[c_\alpha, K]\; e^{-\frac{\tau}{\hbar}K}\;\rangle_{th} \end{aligned}$$

$$\to \lim_{\tau\to 0^-}\left(-\hbar\,\frac{\partial G_{\alpha,\alpha}(\tau)}{\partial\tau}\right) \;=\; \langle c_\alpha^\dagger \;\; [c_\alpha, K]\;\rangle_{th} = \langle H_0 - \mu N\rangle_{th} + 2\langle H_1\rangle_{th}$$

Using $\lim_{\tau\to 0^-} = \langle\, c_\beta^\dagger\, c_\alpha(\tau)\,\rangle_{th}$ we can exoress $\langle H_0 - \mu N\rangle_{th}$ in terms of $\lim_{\tau\to 0^-} G$