# The Variational Cluster Approximation

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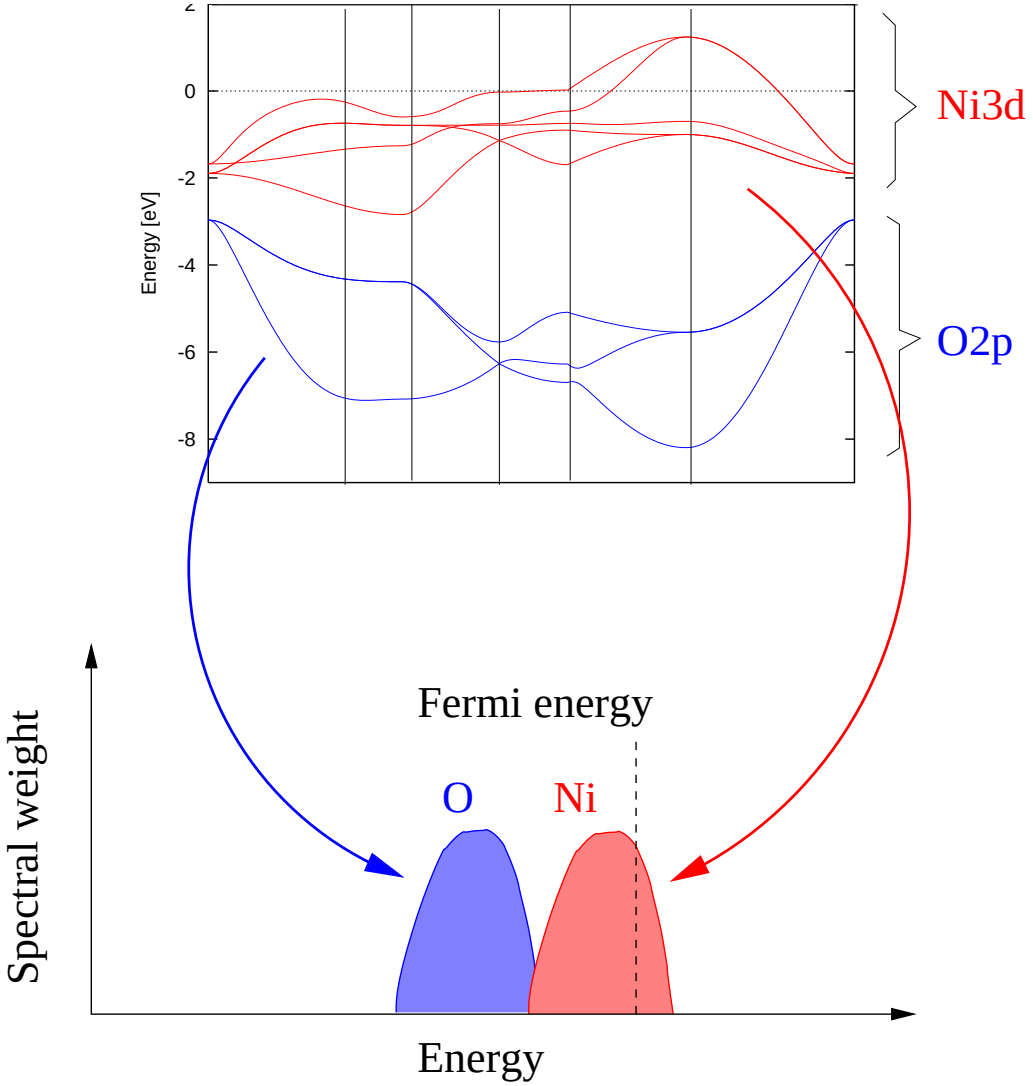
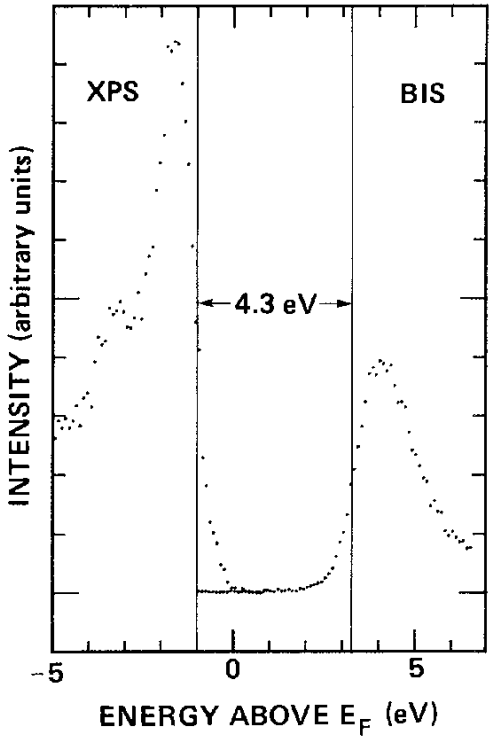
## Introduction

LDA calculations often do not reproduce the single-particle spectra of correlated insulators like NiO



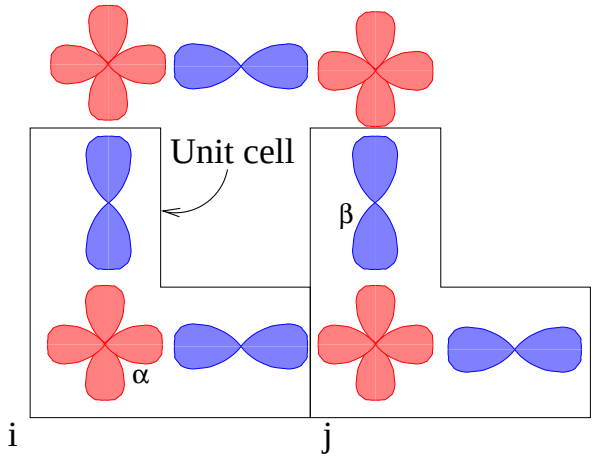




G. A. Sawatzky and J. W. Allen

Phys. Rev. Lett. **53**, 2239 (1984).

# Preliminaries

We consider a solid as a periodic array of orbitals




We introduce Fermion operators $c^\dagger_{i,\alpha}/c_{i,\alpha}$ for electrons in these - $\alpha$ is shorthand for 'orbital type' and spin

The number of orbitals per unit-cell is $n_{orb}$

The Fourier transform of these operators is

$$c^\dagger_{\mathbf{k},\alpha} = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}\cdot(\mathbf{R}_i+\mathbf{r}_\alpha)} \; c^\dagger_{i,\alpha},$$

## Hamiltonian

In terms of these the Hamiltonian reads

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

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

The matrix $\mathbf{t}(\mathbf{k})$ has dimension $2n_{orb} \times 2n_{orb}$ (factor $2$ for spin) and its eigenvalues $E_n(\mathbf{k})$ give the noninteracting band structure

(in the absence of spin-orbit coupling and magnetic field all $E_n(\mathbf{k})$ are twofold degenerate)

## The Green's function

The time ordered imaginary time Green's function is defined as

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

$$c_{i,\alpha}(\tau) \;=\; e^{\tau(H-\mu N)/\hbar}\; c_{i,\alpha}\; e^{-\tau(H-\mu N)/\hbar}$$

It can be shown that this is well defined only for $\tau \in [-\beta\hbar, \beta\hbar]$ and that it is antiperiodic: $\mathbf{G}(\tau+\beta\hbar) = -\mathbf{G}(\tau)$

Accordingly $\mathbf{G}$ can be expanded in a Fourier series with the Matsubara frequencies $\omega_\nu$

$$\mathbf{G}(\tau) \;=\; \frac{1}{\beta\hbar}\sum_{\nu=-\infty}^{\infty} e^{-i\omega_\nu\tau}\;\mathbf{G}(i\omega_\nu)$$

$$\omega_\nu \;=\; \frac{(2\nu+1)\pi}{\beta\hbar}$$

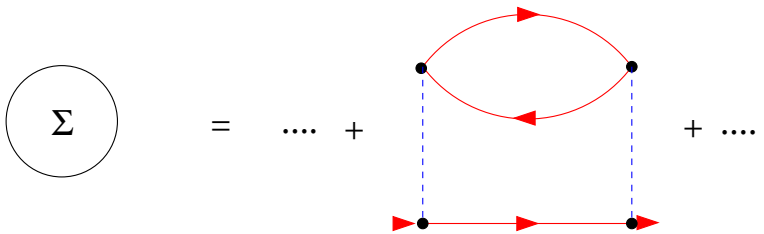
The Fourier transform $\mathbf{G}(\omega)$ is an analytic function in the complex $\omega$-plane with the exception of the real-axis

The poles of $\mathbf{G}(\omega)$ on the real axis give the ionization/affinity energies i.e. the 'quasiparticle band structure'

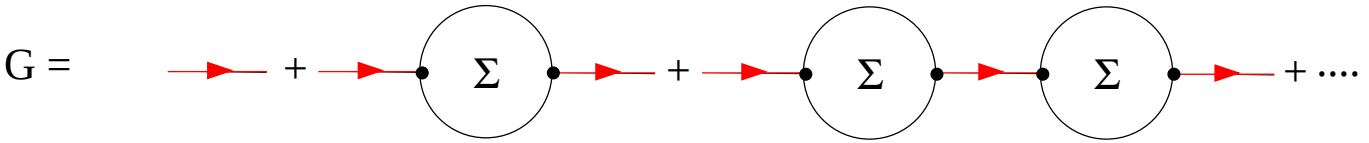
$\mathbf{G}(\omega \pm i0^{+})$ (with $\omega$ real) gives the retarded/advanced real-time Green's function

The imaginary-time Green's function can also be expanded in Feynman diagrams

This allows to introduce the self-energy $\Sigma$ (sum of all one-particle-irreducible diagrams with two 'plugins')...




... and derive the Dyson equation




$$G_{\alpha,\beta} = G^{(0)}_{\alpha,\beta} + G^{(0)}_{\alpha,\mu}\ \Sigma_{\mu,\nu}\ G^{(0)}_{\nu,\beta} + G^{(0)}_{\alpha,\mu}\ \Sigma_{\mu,\nu}\ G^{(0)}_{\nu,\lambda}\ \Sigma_{\lambda,\rho}\ G^{(0)}_{\rho,\beta} + \ldots$$

$$= G^{(0)}_{\alpha,\nu} \left( (1 - \Sigma\ G^{(0)})^{-1} \right)_{\nu,\beta}$$

$$G = (G^{(0)})^{-1} - \Sigma)^{-1}$$

The Dyson equation

$$\mathbf{G}(\mathbf{k},\omega) \;=\; \left(\omega - \frac{1}{\hbar}(\;\mathbf{t}(\mathbf{k}) - \mu\;) - \mathbf{\Sigma}(\mathbf{k},\omega)\right)^{-1}$$

Note: $\mathbf{G}(\mathbf{k},\omega)$, $\mathbf{t}(\mathbf{k})$ and $\mathbf{\Sigma}(\mathbf{k},\omega)$ are matrices of dimension $2n_{orb} \times 2n_{orb}$ - this is a true matrix inversion!

For a single band we can write

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \frac{1}{\hbar}\,(\epsilon_{\mathbf{k}} - \mu) - \Sigma(\mathbf{k},\omega)}$$

The poles of $G(\mathbf{k},\omega)$ give the ionization/affinity energies $\rightarrow$ the equation for the excitation energies thus is

$$\hbar\omega - (\epsilon_{\mathbf{k}} - \mu) = \hbar\Sigma(\mathbf{k},\omega)$$

On the few next pages we omit $\mu$ and $\hbar$ for simplicity then

$$\omega - \epsilon_{\mathbf{k}} = \Sigma(\mathbf{k},\omega)$$

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$$\omega - \epsilon_{\mathbf{k}} = \Sigma(\mathbf{k},\omega)$$

Luttinger has shown (J.M. Luttinger, Phys. Rev. **121**, 942 (1961)) that the self-energy has a simple analytic structure (with $\eta$, $\sigma_i$,$\zeta_i$ real, $\sigma_i > 0$)

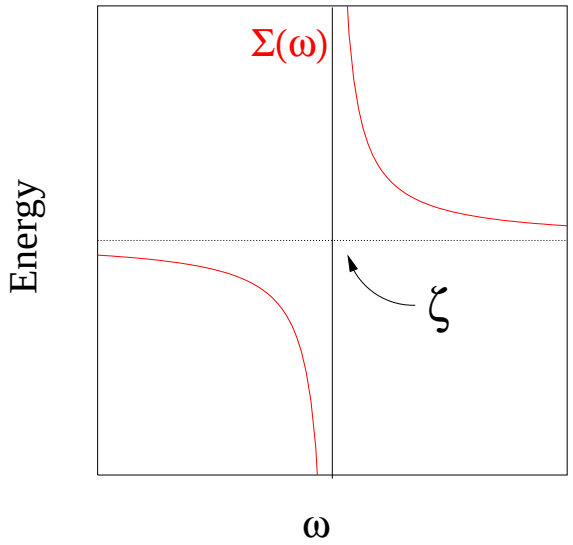
$$\Sigma(\omega) = \eta + \sum_i \frac{\sigma_i}{\omega - \zeta_i}$$

A real constant (='potential') plus a sum of terms which have poles on the real axis

To see the implications of this let us consider just a single pole:

$$\Sigma(\omega) = \frac{\sigma}{\omega - \zeta}$$

The equation for poles of the Green's function (=energies of electron states) reads: $\omega - \epsilon_{\mathbf{k}} = \Sigma(\omega)$



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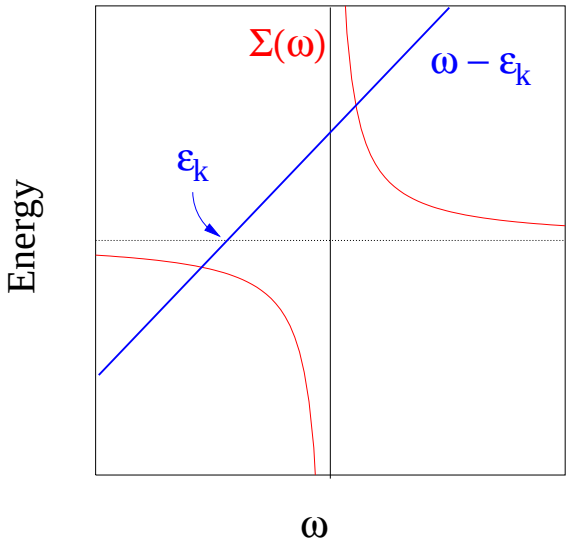

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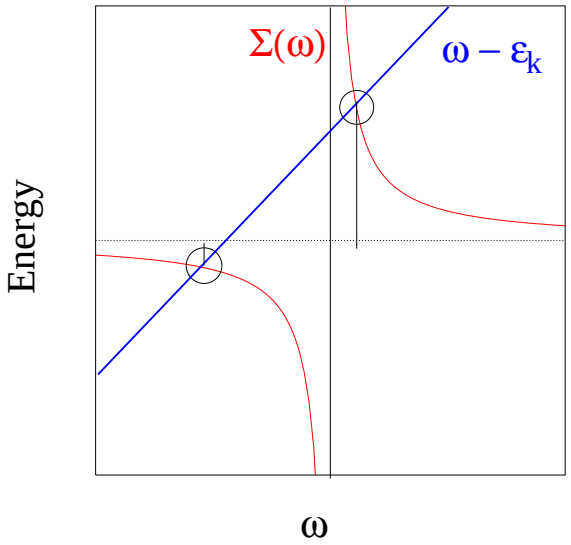

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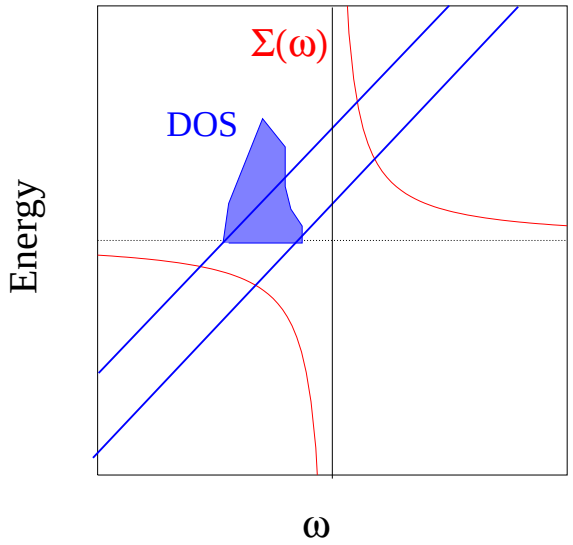

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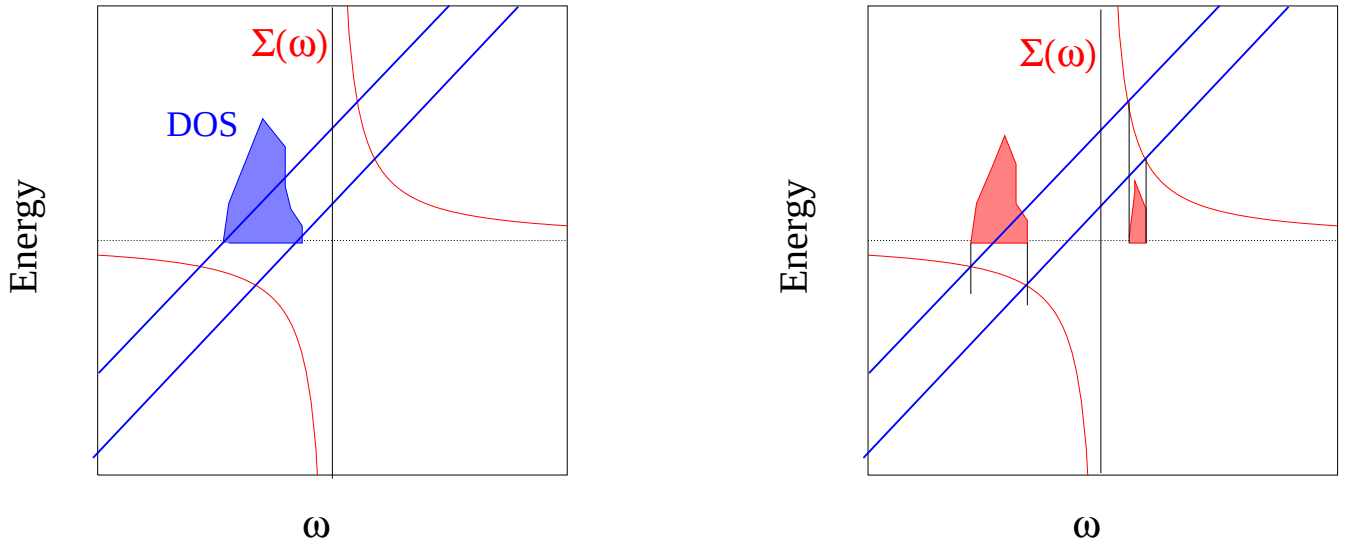
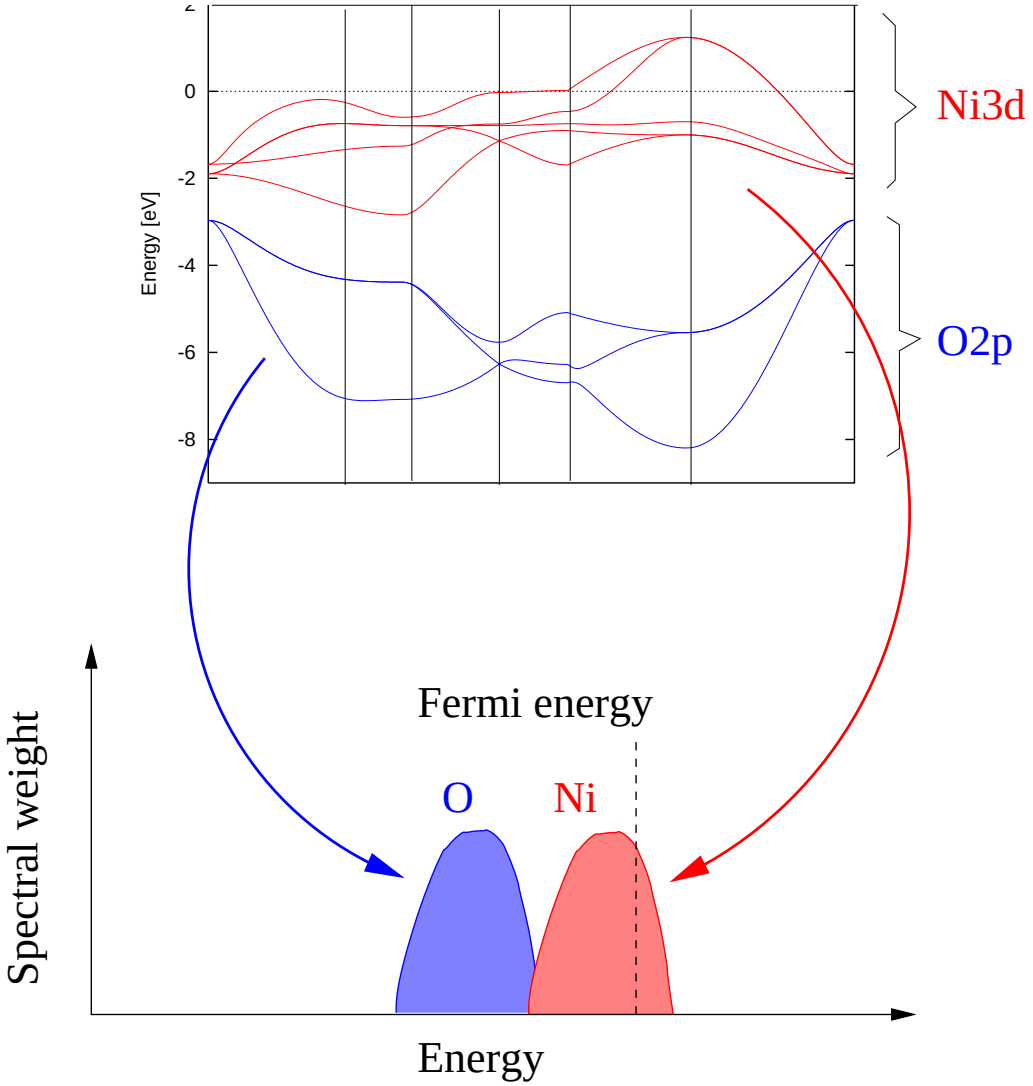
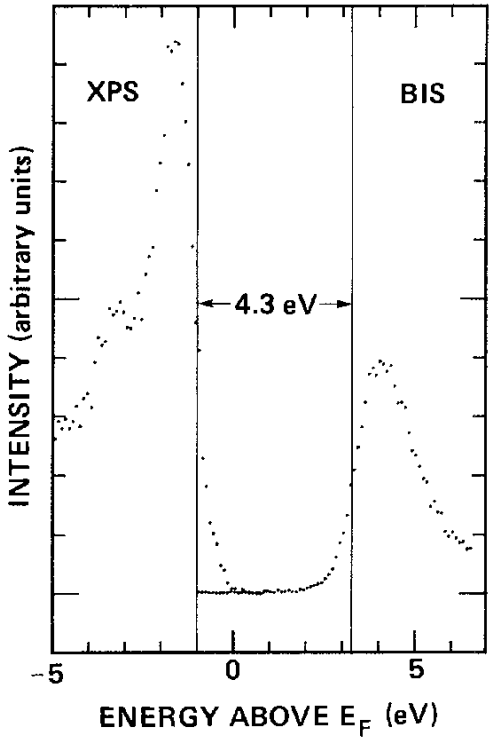


# Reminder: Band Theory vs Experiment

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A self-energy with a single strong pole could resolve a good deal of the discrepancy

## Outline

In 1961 Luttinger and Ward prooved a famous theorem which is the basis of many important developments in the field theory of condensed matter systems

They showed that the Grand Canonical Potential $\Omega$ of an interacting Fermi system can be expressed as a functional of its self-energy $\Sigma$ which is stationary with respect to variations of $\Sigma$ at the exact $\Sigma$

When we apply this theorem for actual calculations we face a similar situation as in density functional theory:

| Density functional theory | Self-energy functional theory |
|---|---|
| $E_0 = E_0[\rho]$ | $\Omega = \Omega[\Sigma]$ |
| $\frac{\delta E_0}{\delta \rho} = 0$ | $\frac{\delta \Omega}{\delta \Sigma} = 0$ |

In both cases the actual form of the functional is unknown (or impossible to actually evaluate)

In both cases one must therefore find a way to 'evaluate' the functional at least approximately

In the case of Self-energy functional theory one way to do this is the Variational Cluster Approximation invented by M. Potthoff (Eur. Phys. J. B $\mathbf{32}$, 429 (2003))

# The Grand Canonical Potential

The Grand Canonical Potential $\Omega$ is defined in terms of the Grand Partition Function $Z$

$$\begin{aligned} \Omega &= -\frac{1}{\beta}\, log(Z) \\ Z &= \text{trace}\, \left(e^{-\beta(\hat{H}-\mu\hat{N})}\right) \end{aligned}$$

- $\hat{H}$: Hamiltonian, $\hat{N}$ operator of particle number
- $\beta = 1/(k_B T)$
- $k_B$: Boltzmann constant, $T$: Temperature, $\mu$: chemical potential

If we know a complete set of eigenstates $|i\rangle$

$$\begin{aligned} \hat{H}|i\rangle &= E_i|i\rangle \\ \hat{N}|i\rangle &= N_i|i\rangle \end{aligned}$$

we obtain

$$Z = \sum_i e^{-\beta(E_i-\mu N_i)}$$

## $\Omega$ can be evaluated analytically for some systems

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: $C_v \propto T$

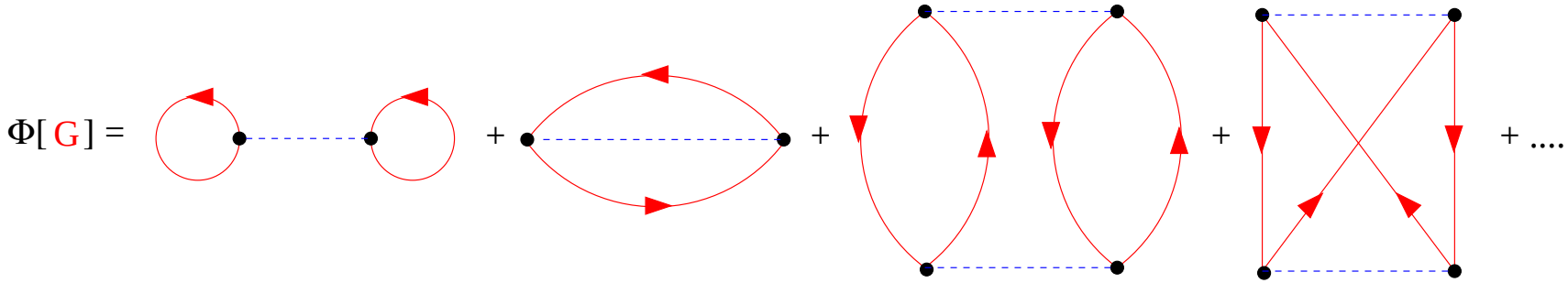
But: No way to calculate this for an interacting system of macroscopic size

## 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))

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

- $\omega_\nu = \frac{(2\nu+1)\pi}{\hbar\beta}$: Matsubara Frequencies
- $\mathbf{G}$: 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 $H \rightarrow H_0 + \lambda H_1$
- 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 $\Omega'$ and $\Omega$

## 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

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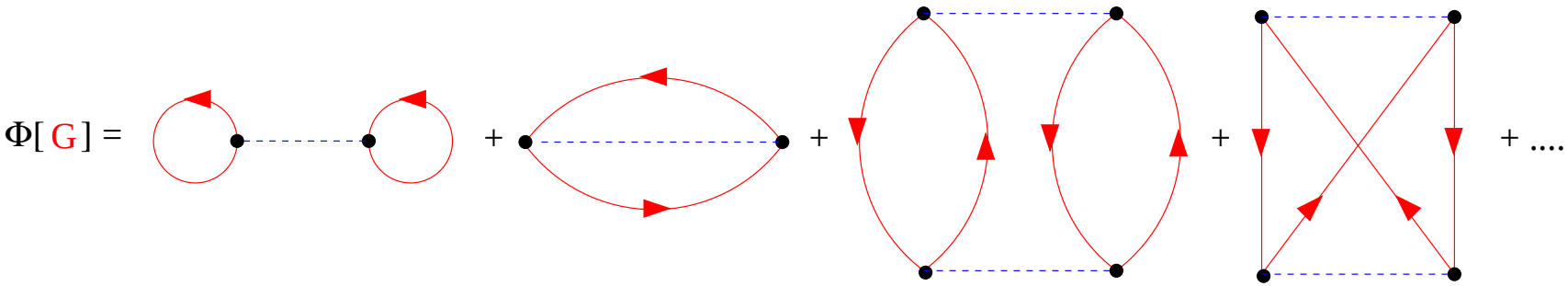
For noninteracting electrons we have $\boldsymbol{\Sigma} = 0$ and $\Phi = 0$:



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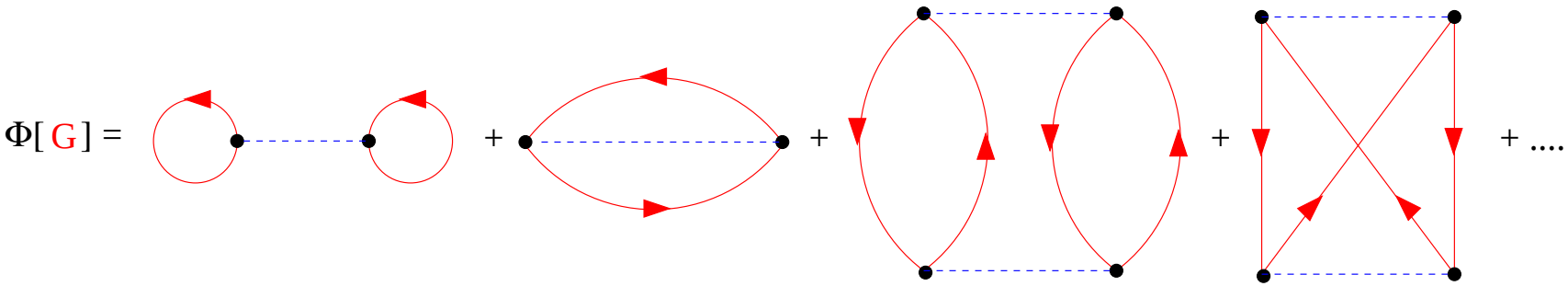

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Theorem: The determinant of a matrix $A$ is equal to the product of its eigenvalues $a_n$

$$\det A=\prod_n a_n \;\rightarrow\; \ln\;\det A=\sum_n \ln(a_n)$$

For noninteracting Fermions we have

$$\mathbf{G}^{-1}(\mathbf{k},\omega) \;=\; \omega-\frac{1}{\hbar}\left(\;\mathbf{t}(\mathbf{k})\;\;-\mu\;\right)$$

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$$\rightarrow\Omega' \;=\; -\lim_{\eta\to 0^+}\frac{1}{\beta}\sum_{\mathbf{k},\nu} e^{i\omega_\nu\eta}\sum_{n=1}^{2n_{orb}}\ln\left(\,-i\omega_\nu+\frac{1}{\hbar}\left(\,E_n(\mathbf{k})-\mu\,\right)\right)$$

## Intermezzo: Sum over Matsubara-frequencies

Consider the Fermi function

$$f(\omega) \;=\; \frac{1}{e^{\beta\hbar\omega}+1}$$

This has a pole (zero of the denominator) if $e^{\beta\hbar\omega} = -1$ or $\beta\hbar\omega = i\pi + \nu \cdot 2\pi i$ ($\nu$ integer) or

$$\omega \;=\; i\,\frac{(2\nu+1)\pi}{\beta\hbar} = i\omega_\nu$$

The Fermi function has poles at all Matsubara frequencies

To obtain the residuum: set $\omega = i\omega_\nu + z$

$$\begin{aligned} f(\omega) \;&=\; \frac{1}{e^{\beta\hbar\omega}+1} \\ &=\; \frac{1}{e^{i\beta\hbar\omega_\nu}\; e^{\beta\hbar z}+1} \\ &=\; \frac{1}{(-1)\;(1+\beta\hbar z)+1} \\ &=\; -\frac{1}{\beta\hbar}\,\frac{1}{z} \end{aligned}$$

All poles have the same residuum: $-1/\beta\hbar$

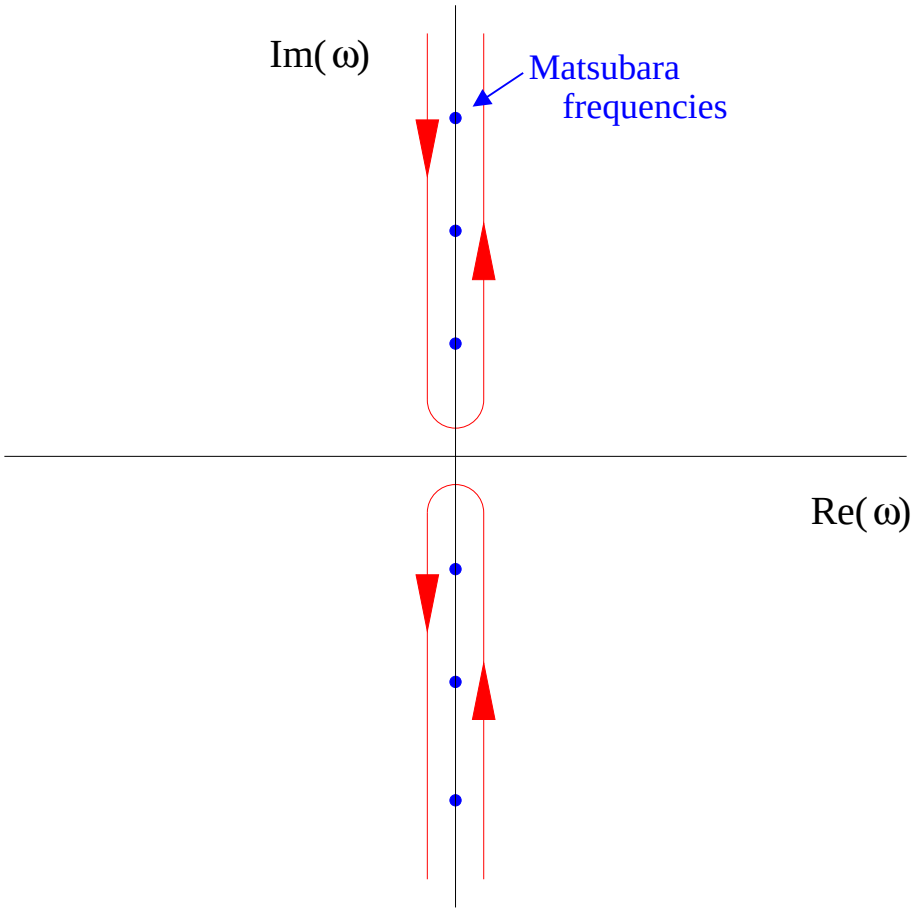
## Intermezzo: Sum over Matsubara-frequencies

The Fermi function $f(\omega)$ has poles at all Matsubara frequencies $i\omega_\nu$ each with residuum $-1/\beta\hbar$

Therefore if $g(\omega)$ is an analytic function

$$\oint_C d\omega\ f(\omega)\ g(\omega) \ = \ 2\pi i \ \sum_\nu \ (-\frac{1}{\beta\hbar})\ g(i\omega_\nu)$$

$$\rightarrow -\frac{1}{\beta} \ \sum_\nu \ g(i\omega_\nu) \ = \ \frac{\hbar}{2\pi i} \ \oint_C \ d\omega\ f(\omega)\ g(\omega)$$



We had

$$\Omega' \;=\; -\lim_{\eta\to 0^+}\;\frac{1}{\beta}\sum_{\nu}\sum_{\mathbf{k}}\;e^{i\omega_\nu\eta}\sum_{n=1}^{2n_{orb}}\ln\left(\;-i\omega_\nu+\frac{1}{\hbar}\left(\;E_n(\mathbf{k})-\mu\;\right)\right)$$

Now use

$$-\frac{1}{\beta}\sum_{\nu}\;g(i\omega_\nu)\;=\;\frac{\hbar}{2\pi i}\oint_{\mathcal{C}}d\omega\;f(\omega)\;g(\omega)$$

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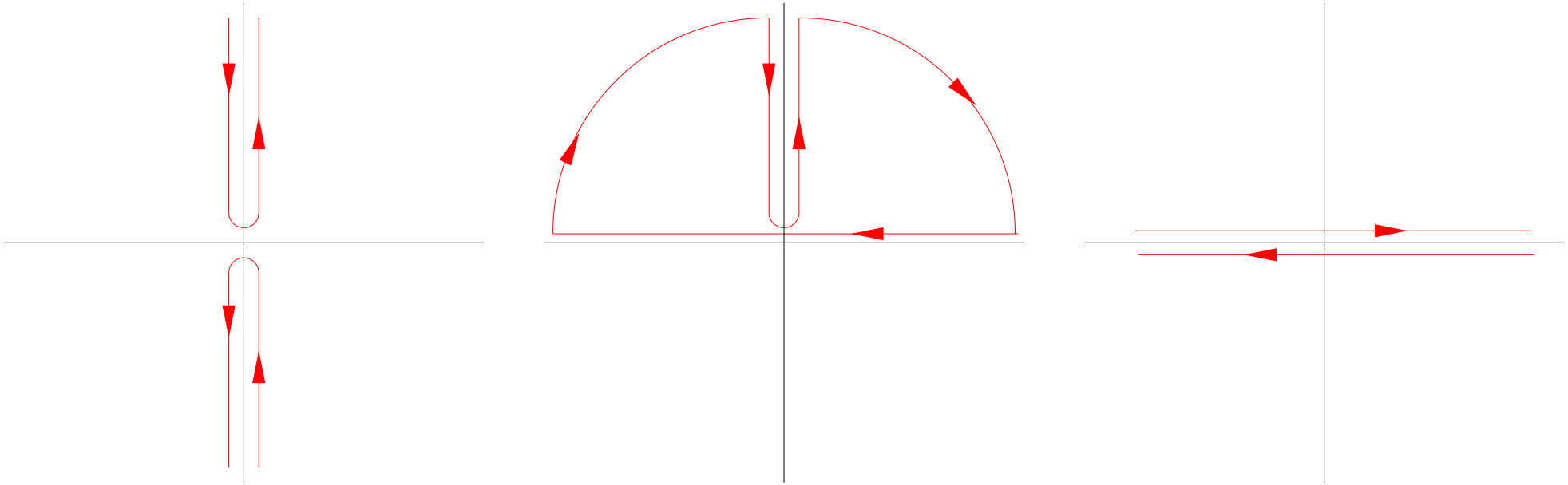
$$-\frac{1}{\beta}\sum_{\nu} g(i\omega_\nu) \;=\; \frac{\hbar}{2\pi i}\oint_{\mathcal{C}} d\omega\; f(\omega)\; g(\omega)$$

and obtain

$$\Omega' \;=\; \lim_{\eta\to 0^+}\frac{\hbar}{2\pi i}\oint_{\mathcal{C}} d\omega\; f(\omega)\sum_{\mathbf{k}} e^{\omega\eta}\sum_{n=1}^{2n_{orb}}\ln\left(\,-\omega+\frac{1}{\hbar}\left(\,E_n(\mathbf{k})-\mu\,\right)\right)$$

# Deforming the Contour

Consider the following three contours:



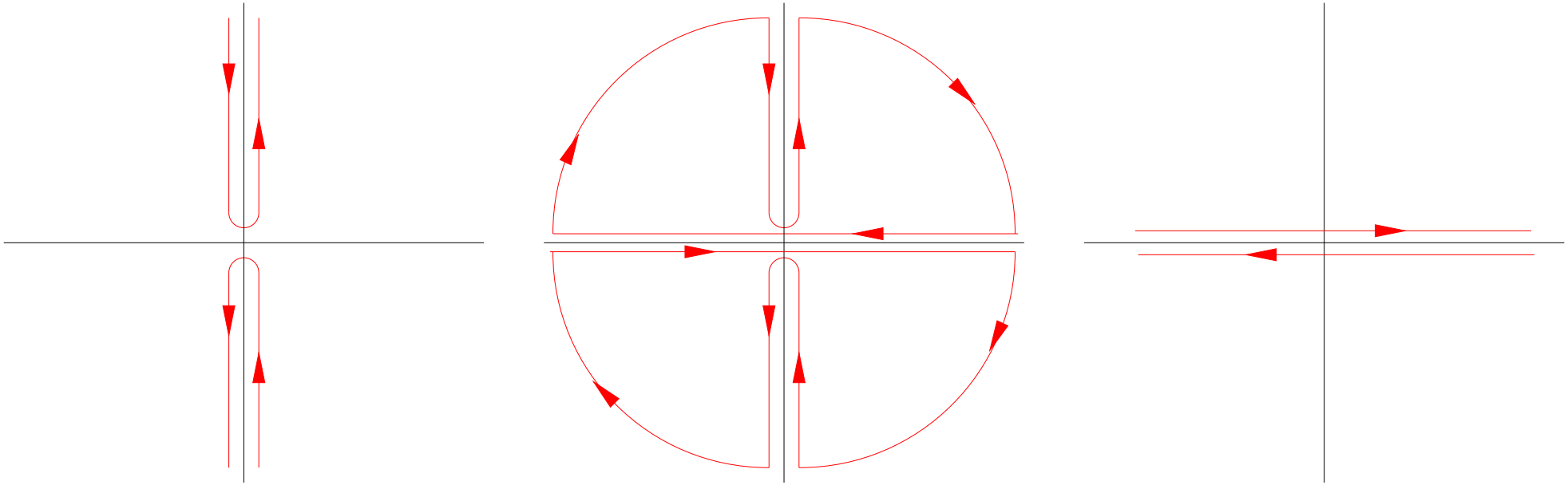
The integrand

$$f(\omega)\, e^{\omega\eta} \sum_{\mathbf{k}} \sum_{n=1}^{2n_{orb}} \ln\left( -\omega + \frac{1}{\hbar}\left( E_n(\mathbf{k}) - \mu \right) \right)$$

The integral along the closed contour vanishes

# Deforming the Contour

Consider the following three contours:



The integrand

$$f(\omega)\, e^{\omega\eta} \sum_{\mathbf{k}} \sum_{n=1}^{2n_{orb}} \ln\left( -\omega + \frac{1}{\hbar}\left( E_n(\mathbf{k}) - \mu \right) \right)$$

The integral along the closed contour vanishes

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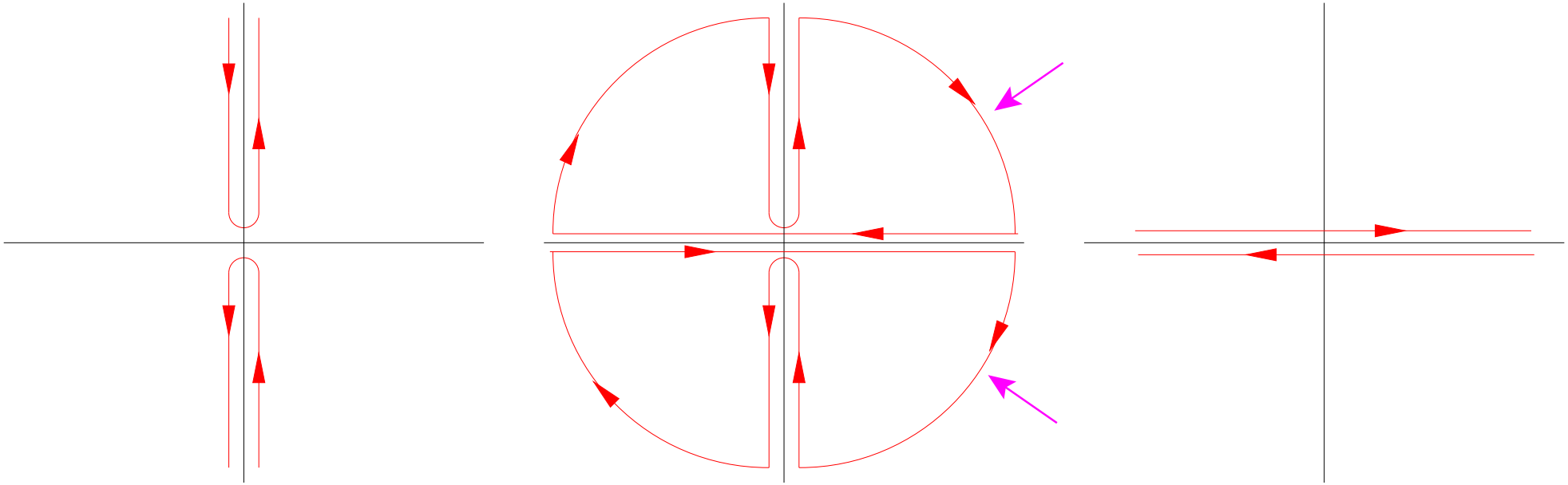

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The integral along the right arc vanishes

$$f(\omega) = \frac{1}{e^{\beta\hbar\omega} + 1} \;\propto\; e^{-\beta\hbar\, \Re\omega}$$

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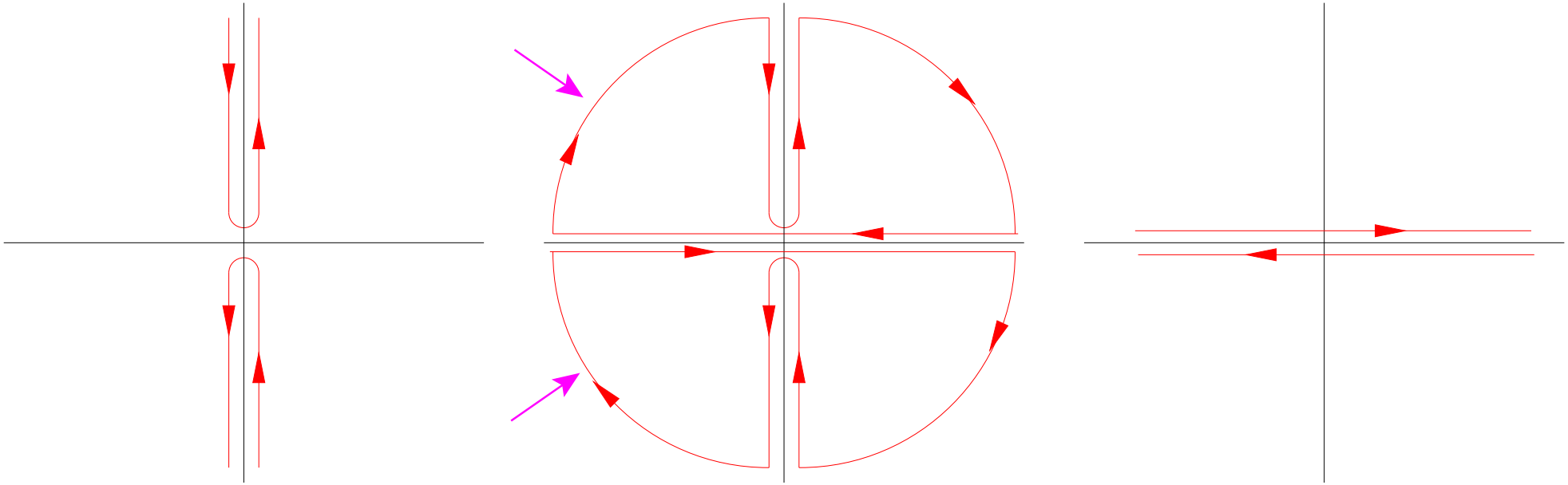

The integrand

$$f(\omega)\, e^{\omega\eta} \sum_{\mathbf{k}} \sum_{n=1}^{2n_{orb}} \ln\left( -\omega + \frac{1}{\hbar}\left( E_n(\mathbf{k}) - \mu \right) \right)$$

The integral along the left arc vanishes

$$\propto e^{-\eta|\Re\omega|}$$

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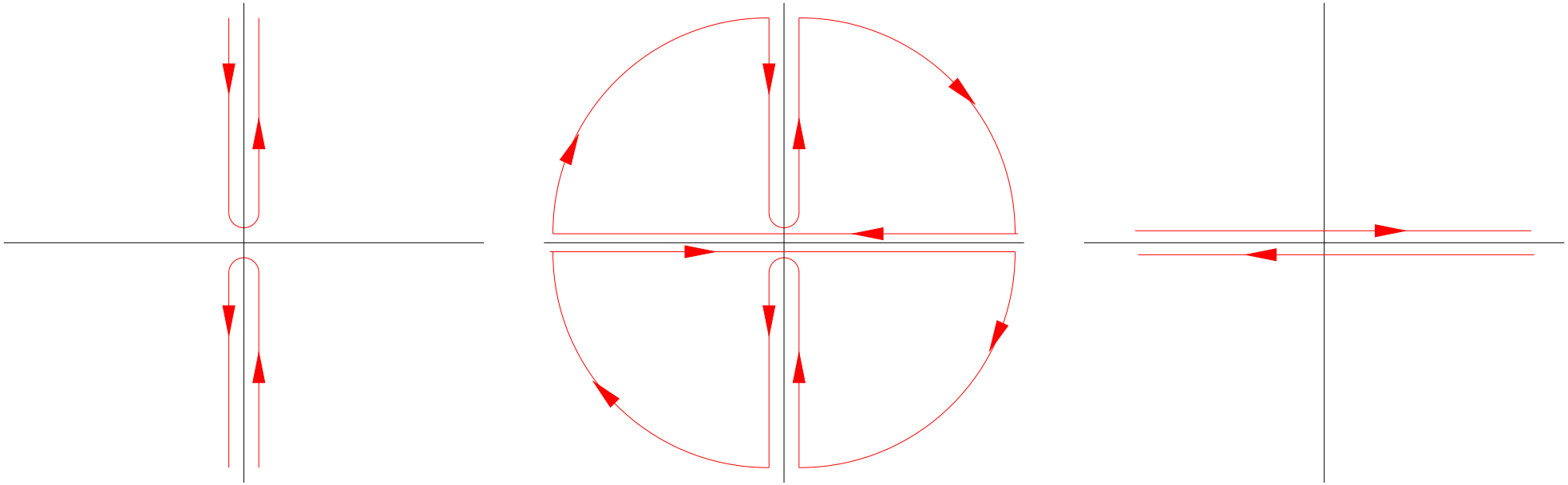

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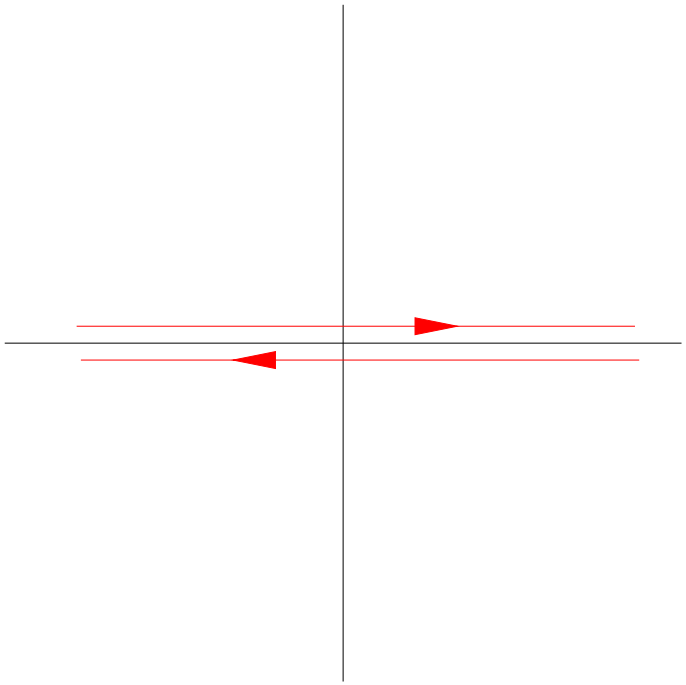
$$\rightarrow \oint_{\mathcal{C}} d\omega \cdots = \oint_{\mathcal{C}'} d\omega$$

We now have

$$\Omega' \;=\; \lim_{\eta\to 0^+} \sum_{\mathbf{k}} \frac{\hbar}{2\pi i} \oint_{\mathcal{C}'} d\omega \; f(\omega)\, e^{\omega\eta} \sum_{n=1}^{2n_{orb}} \ln\left( -\omega + \frac{1}{\hbar}\left( E_n(\mathbf{k}) - \mu \right) \right)$$



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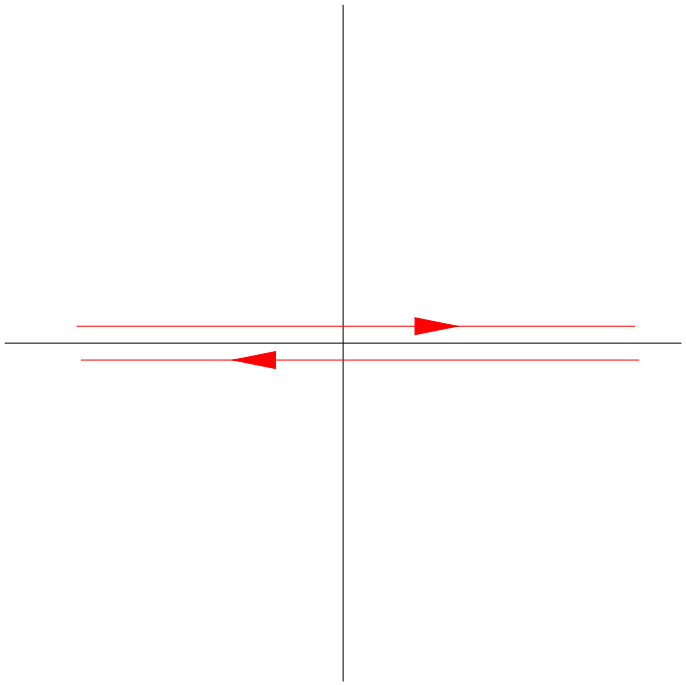

Next we use

$$f(\omega) \;=\; -\frac{1}{\beta\hbar}\,\frac{d}{d\omega}\ln\left(1+e^{-\beta\hbar\omega}\right)$$

$$=\; -\frac{1}{\beta\hbar}\,\frac{-\beta\hbar\, e^{-\beta\hbar\omega}}{1+e^{-\beta\hbar\omega}}$$

and integrate by parts

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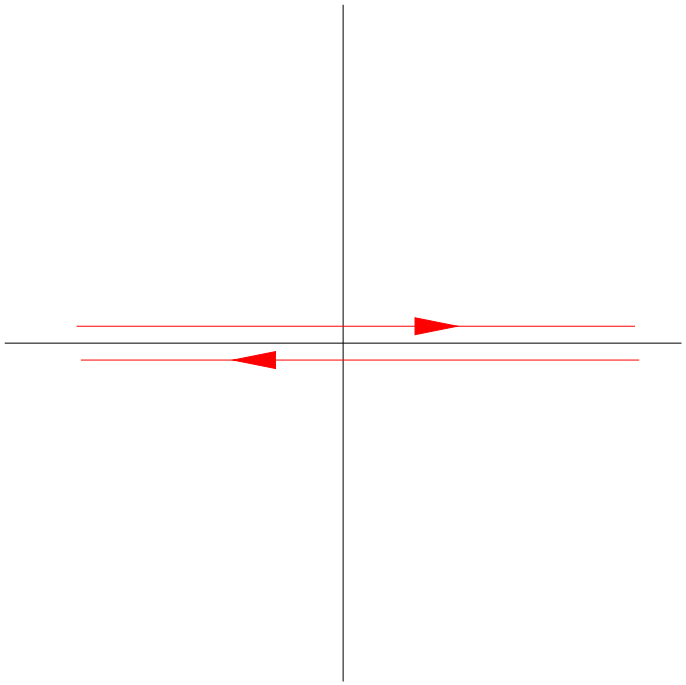
$$\Omega' \;=\; \lim_{\eta\to 0^+} \sum_{\mathbf{k}} \frac{\hbar}{2\pi i} \oint_{\mathcal{C}'} d\omega \; f(\omega)\; e^{\omega\eta} \sum_{n=1}^{2n_{orb}} \ln\left( -\omega + \frac{1}{\hbar}\left( E_n(\mathbf{k}) - \mu \right) \right)$$



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and integrate by parts

$$\Omega' \;=\; \frac{1}{\beta}\,\lim_{\eta\to 0^+} \sum_{\mathbf{k}} \frac{1}{2\pi i} \oint_{\mathcal{C}'} d\omega \,\ln\left(1+e^{-\beta\hbar\omega}\right) \frac{d}{d\omega}\left[ e^{\omega\eta} \sum_{n=1}^{2n_{orb}} \ln\left( -\omega + \frac{1}{\hbar}\left( E_n(\mathbf{k}) - \mu \right) \right)\right]$$

We had

$$\Omega' = \frac{1}{\beta} \lim_{\eta \to 0^+} \sum_{\mathbf{k}} \frac{1}{2\pi i} \oint_{\mathcal{C}'} d\omega \ \ln\left(1 + e^{-\beta\hbar\omega}\right) \ \frac{d}{d\omega} \left[ e^{\omega\eta} \sum_{n=1}^{2n_{orb}} \ln\left( -\omega + \frac{1}{\hbar} \left( \ E_n(\mathbf{k}) - \mu \ \right) \right) \right]$$

$$= \lim_{\eta \to 0^+} \frac{1}{\beta} \frac{1}{2\pi i} \sum_{\mathbf{k}} \sum_{n=1}^{2n_{orb}} \oint_{\mathcal{C}'} d\omega \ \ln(1 + e^{-\beta\hbar\omega}) \ e^{\eta\omega} \ \frac{1}{\omega - \frac{1}{\hbar}(E_n(\mathbf{k}) - \mu)} + 0(\eta)$$

We had

$$\Omega' = \frac{1}{\beta} \lim_{\eta \to 0^+} \sum_{\mathbf{k}} \frac{1}{2\pi i} \oint_{\mathcal{C}'} d\omega \ \ln\left(1 + e^{-\beta\hbar\omega}\right) \ \frac{d}{d\omega} \left[ e^{\omega\eta} \sum_{n=1}^{2n_{orb}} \ln\left( -\omega + \frac{1}{\hbar}\left( E_n(\mathbf{k}) - \mu \right) \right) \right]$$

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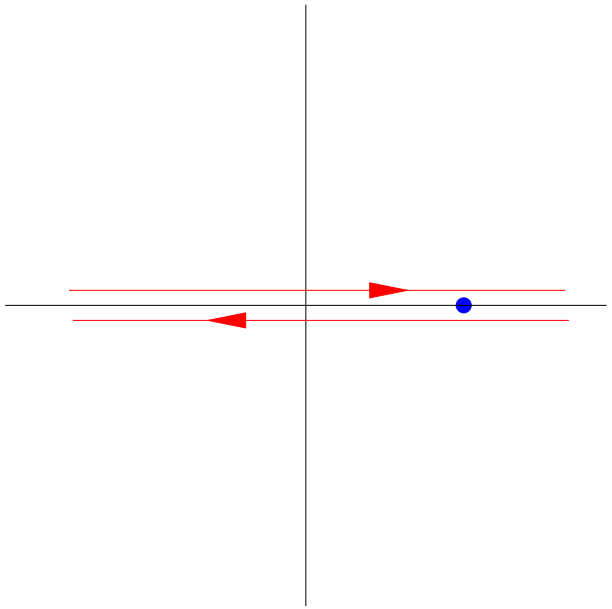

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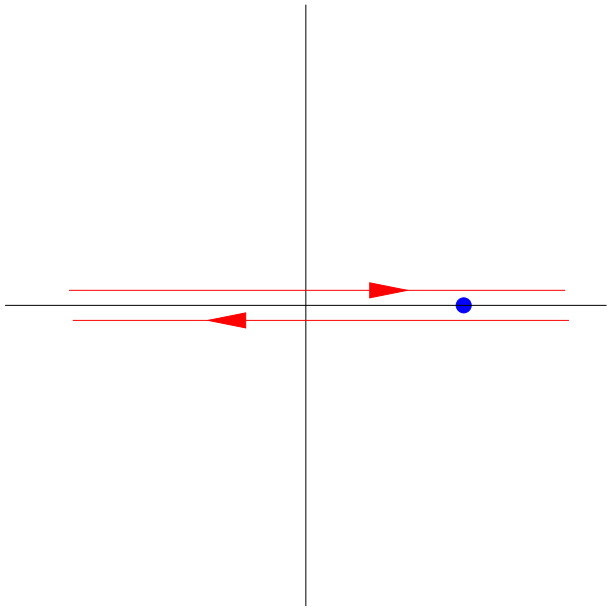

Equation for pole: $\hbar\omega_{pole} = E_n(\mathbf{k}) - \mu$

$\rightarrow$ Residuum is

$$\ln\left(1+e^{-\beta\hbar\omega_{pole}}\right) = \ln\left(1+e^{-\beta(E_n(\mathbf{k})-\mu)}\right)$$

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

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

- We replace $H \rightarrow H_0 + \lambda H_1$
- 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 $\Omega'$ and $\Omega$

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

The definition of $\Omega$

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

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* $\lambda$

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

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

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

Now: Use the Dyson equation

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

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Its Fourier transform is

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

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

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

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

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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

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

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

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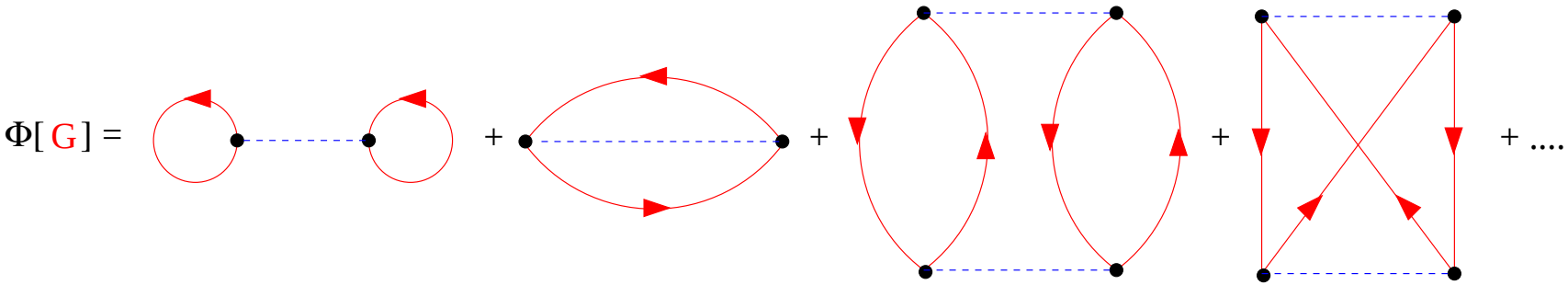
# The Precise Definition and Properties of the Luttinger-Ward Functional $\Phi[\mathbf{G}]$

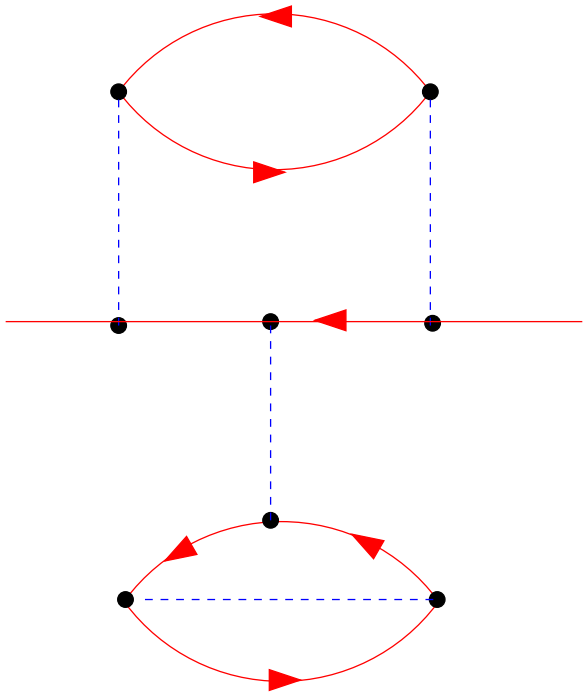
Reminder: The Luttinger-Ward functional is defined in terms of Feynman diagrams



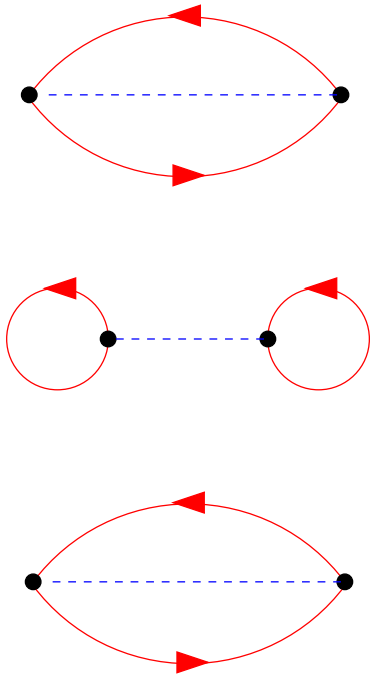

The diagrams which are included into $\Phi$ are

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

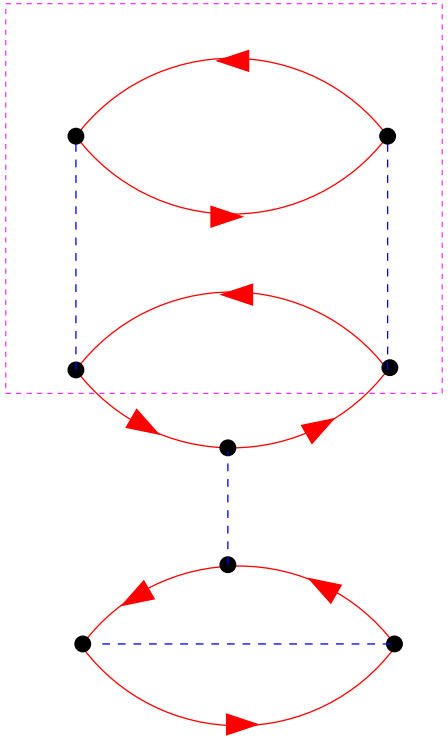
Excluded diagrams



Open ends!

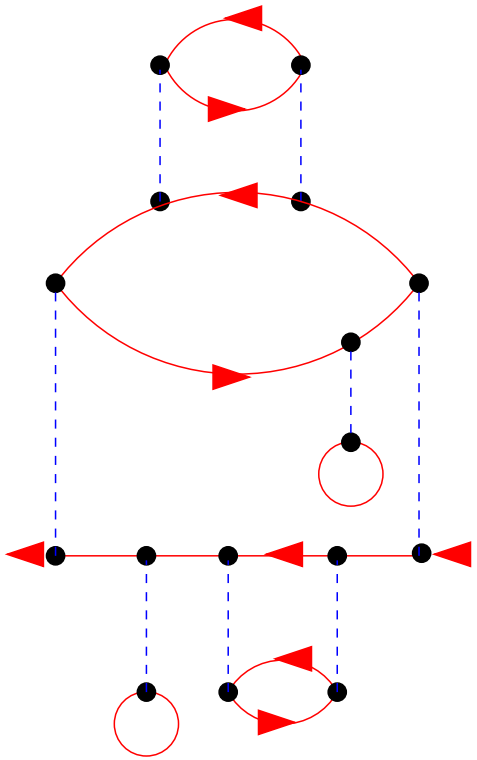


Disconnected!



Self−energy insertion!

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



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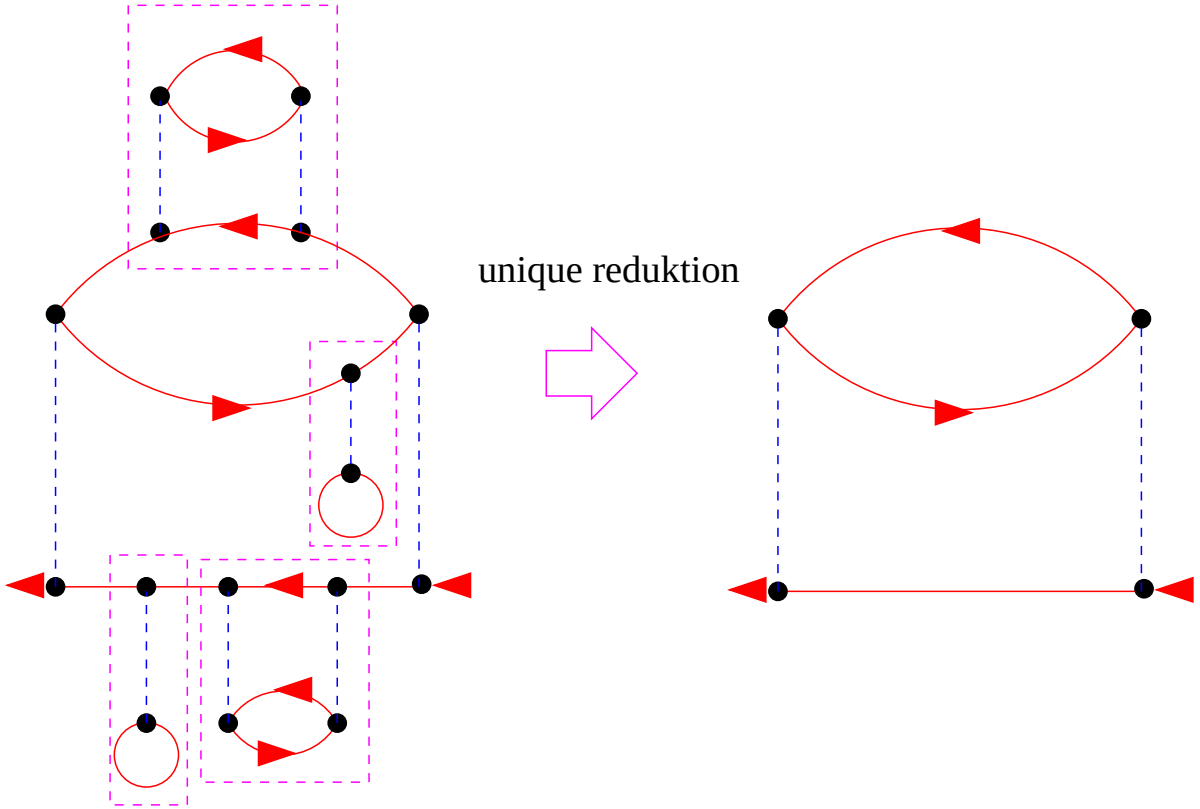
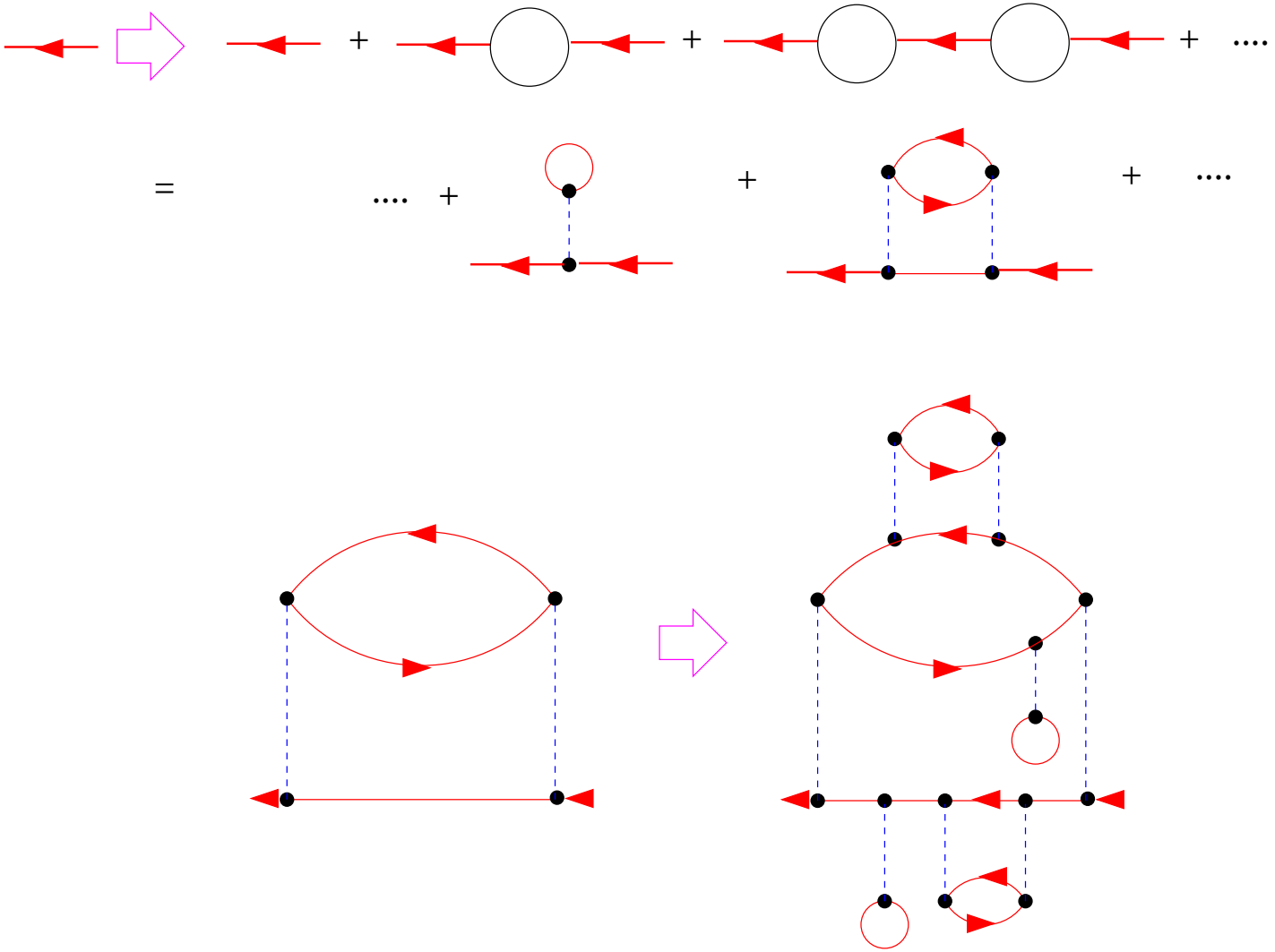



Each self-energy diagram can be reduced uniquely to a skeleton diagram by removing all self-energy insertions

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

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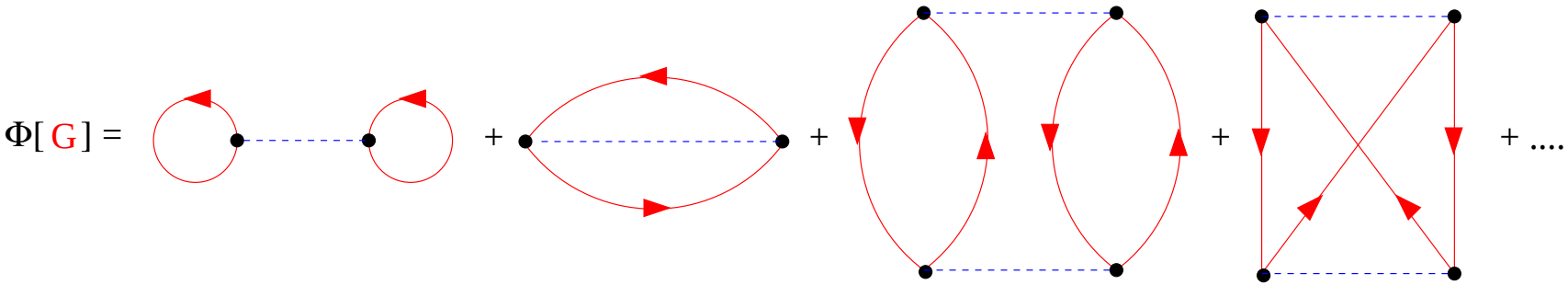


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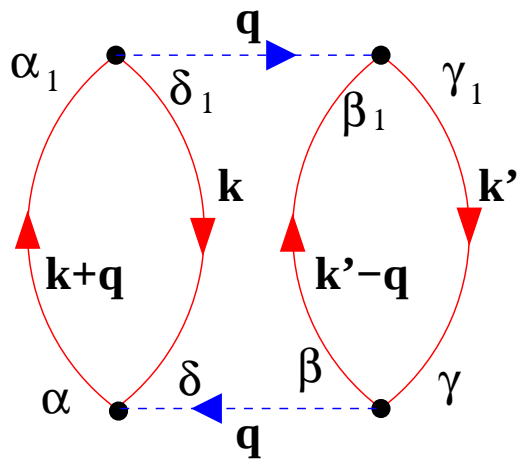
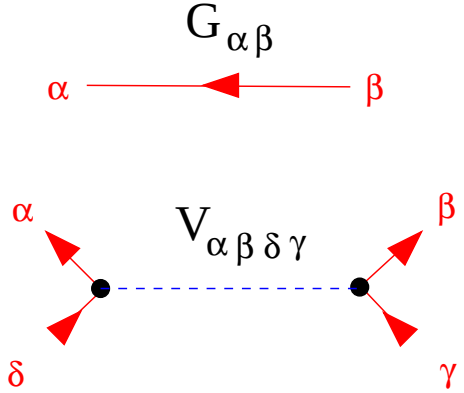
The Diagrams are Converted into Multiple Sums using the Standard Feynman Rules....

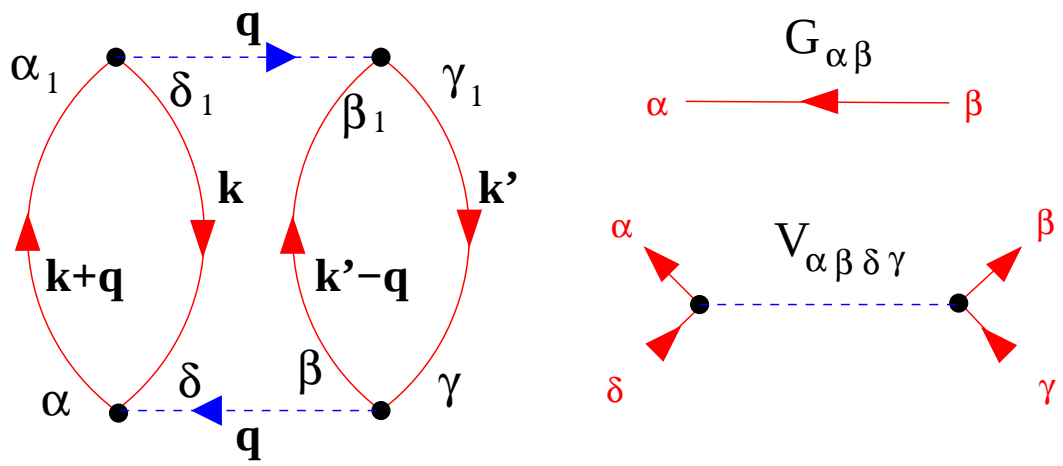



$$\left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma,\delta} \sum_{\alpha_1,\beta_1,\gamma_1,\delta_1} \sum_{\nu,\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{q},-\mathbf{q})$$

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

.... but there is one crucial difference!

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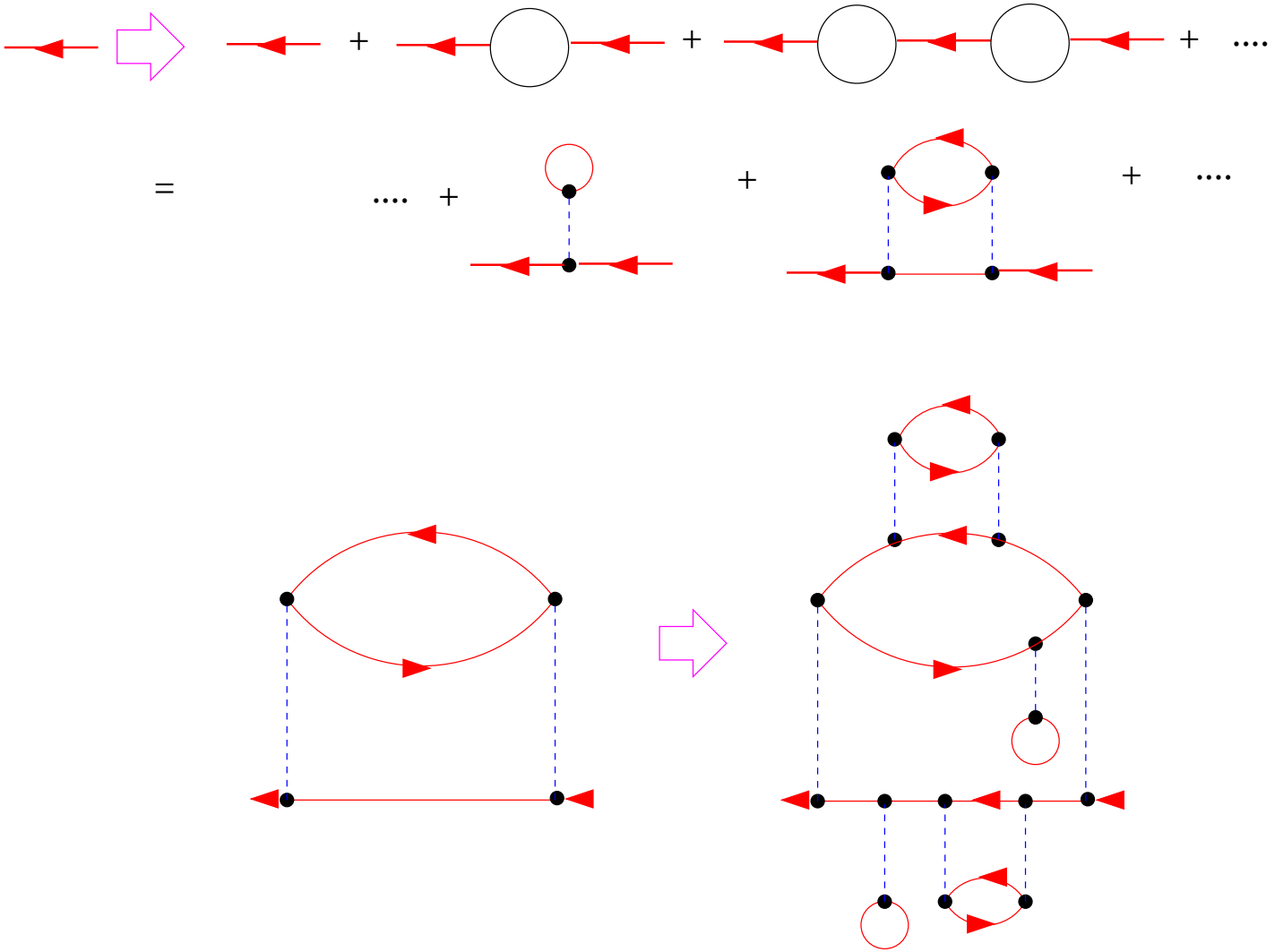
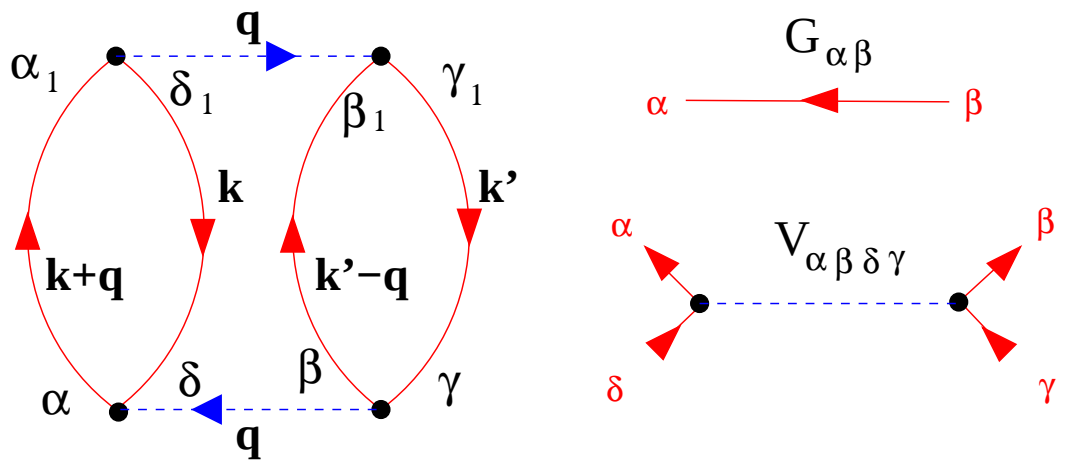
$$G_{\alpha_1,\alpha}(\mathbf{k}+\mathbf{q}, i\omega_\nu+\omega_\mu)\, G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu)\, G_{\beta_1,\beta}(\mathbf{k}'-\mathbf{q}, i\omega_{\nu'}-i\omega_\mu)\, G_{\gamma,\gamma_1}(\mathbf{k}', i\omega_{\nu'})$$

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!



The properties of the system under study enter only at one point




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

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

The only property of the system which enters the functional $\Phi$ therefore are the interactions lines - that means the matrix elements of the interaction

This implies in particular that the elements of the single-particle Hamiltonian $H_0$ appear nowhere in the Luttinger-Ward functional

## Symmetry factors

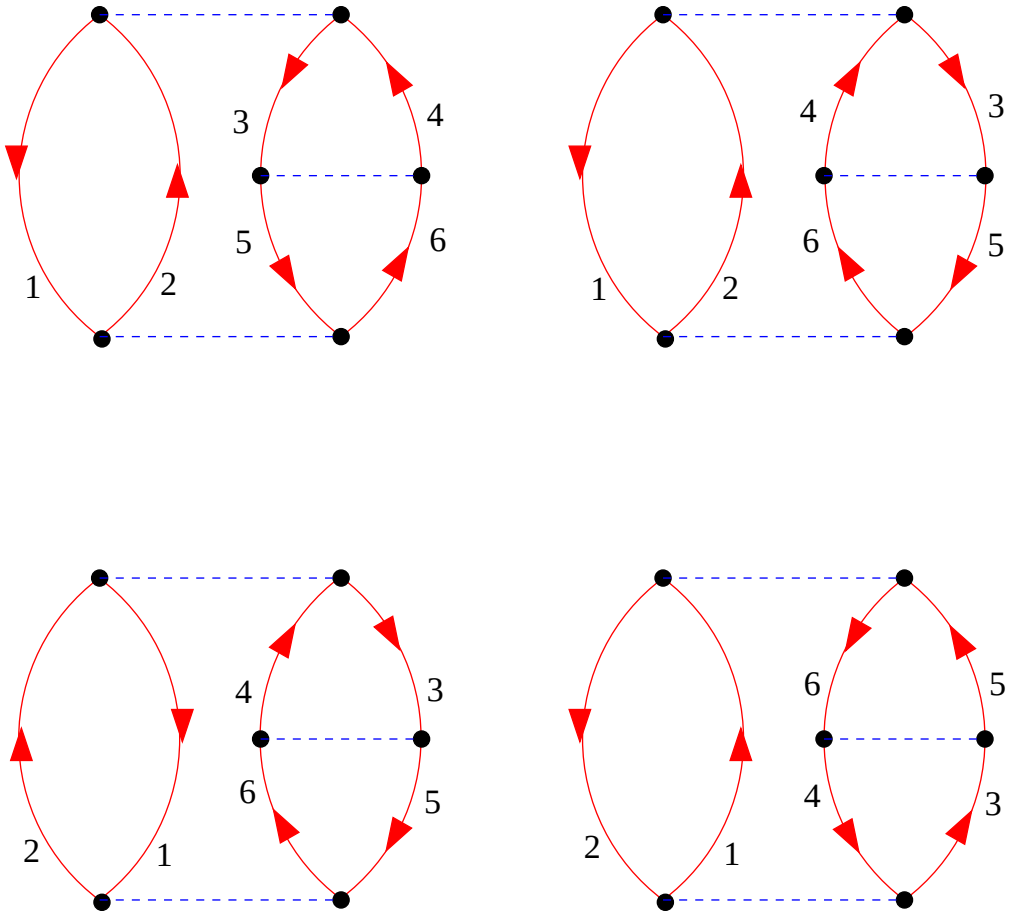
In addition to the factors from the Feynman rules the expression for each diagram is multiplied by

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

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

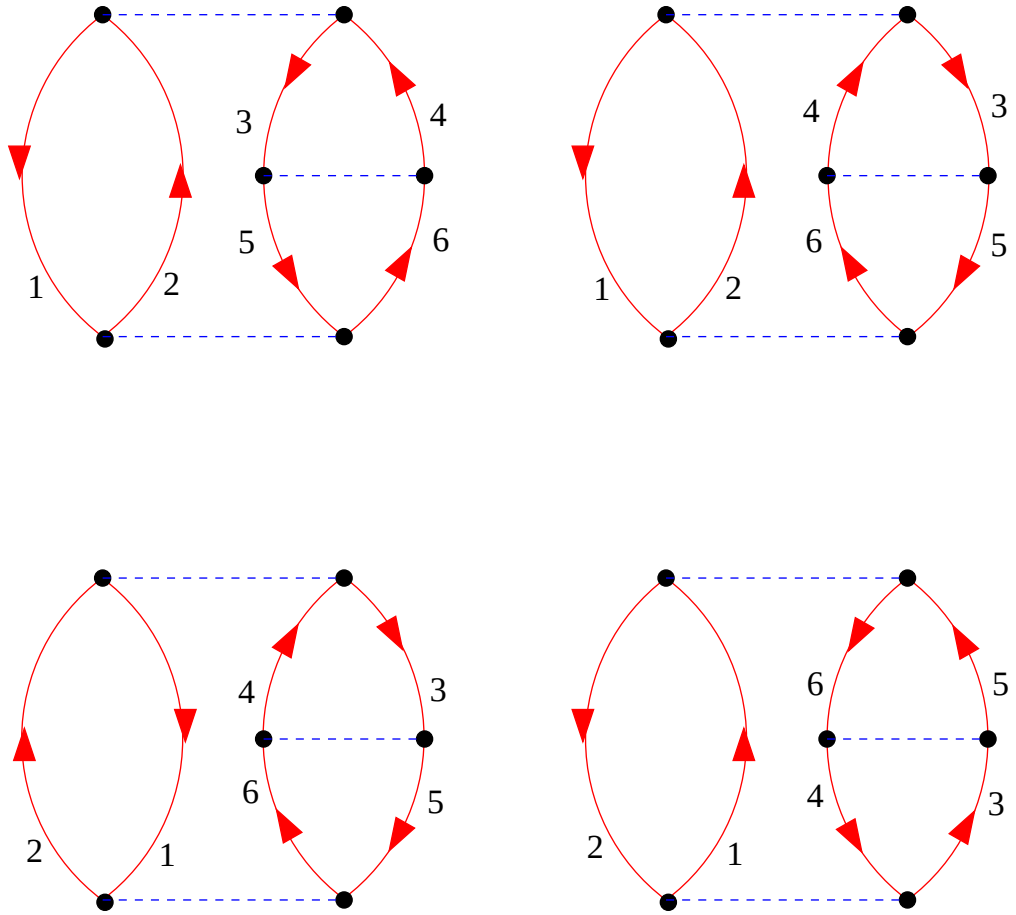



The final diagram looks exactly like the original one - including direction of all arrows - but the Green's function lines are permuted!

## 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

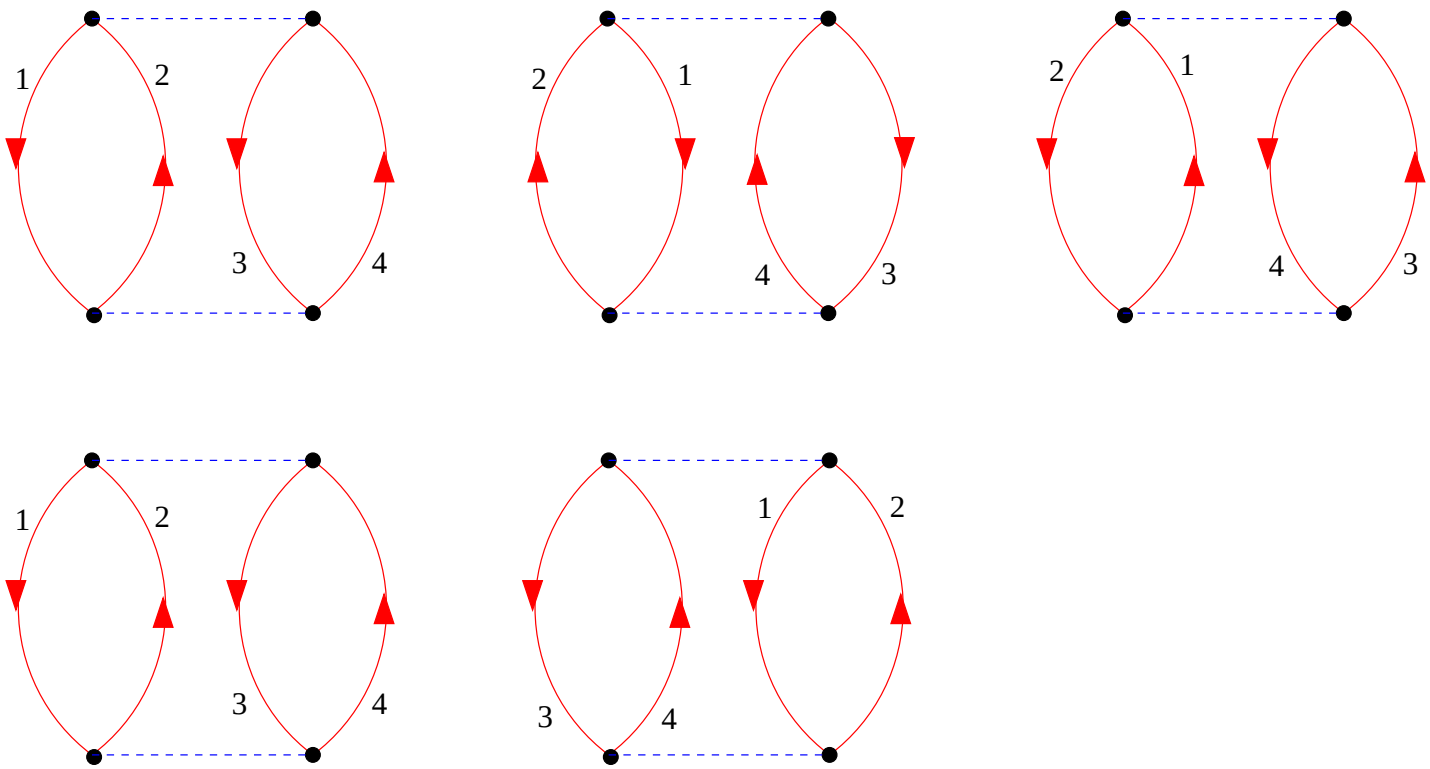
## Example




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 $(4, 5)$

## Another example




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

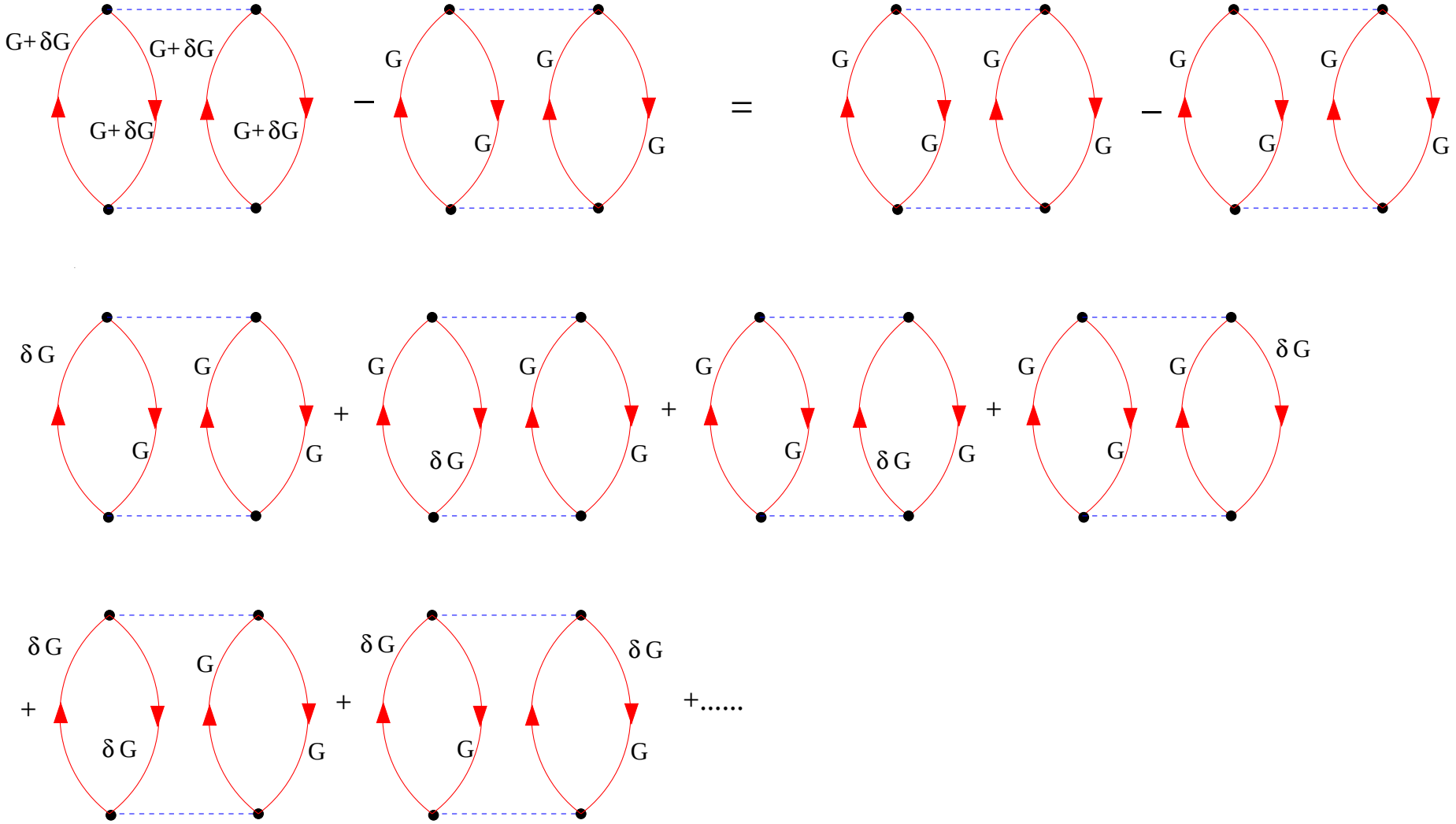
The Luttinger-Ward functional is the generating functional of the self-energy

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

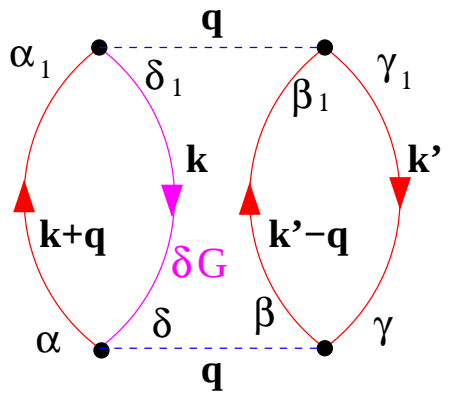
To see this we need to consider the change of a given diagram contributing to $\Phi$ under a change of $G$:

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

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



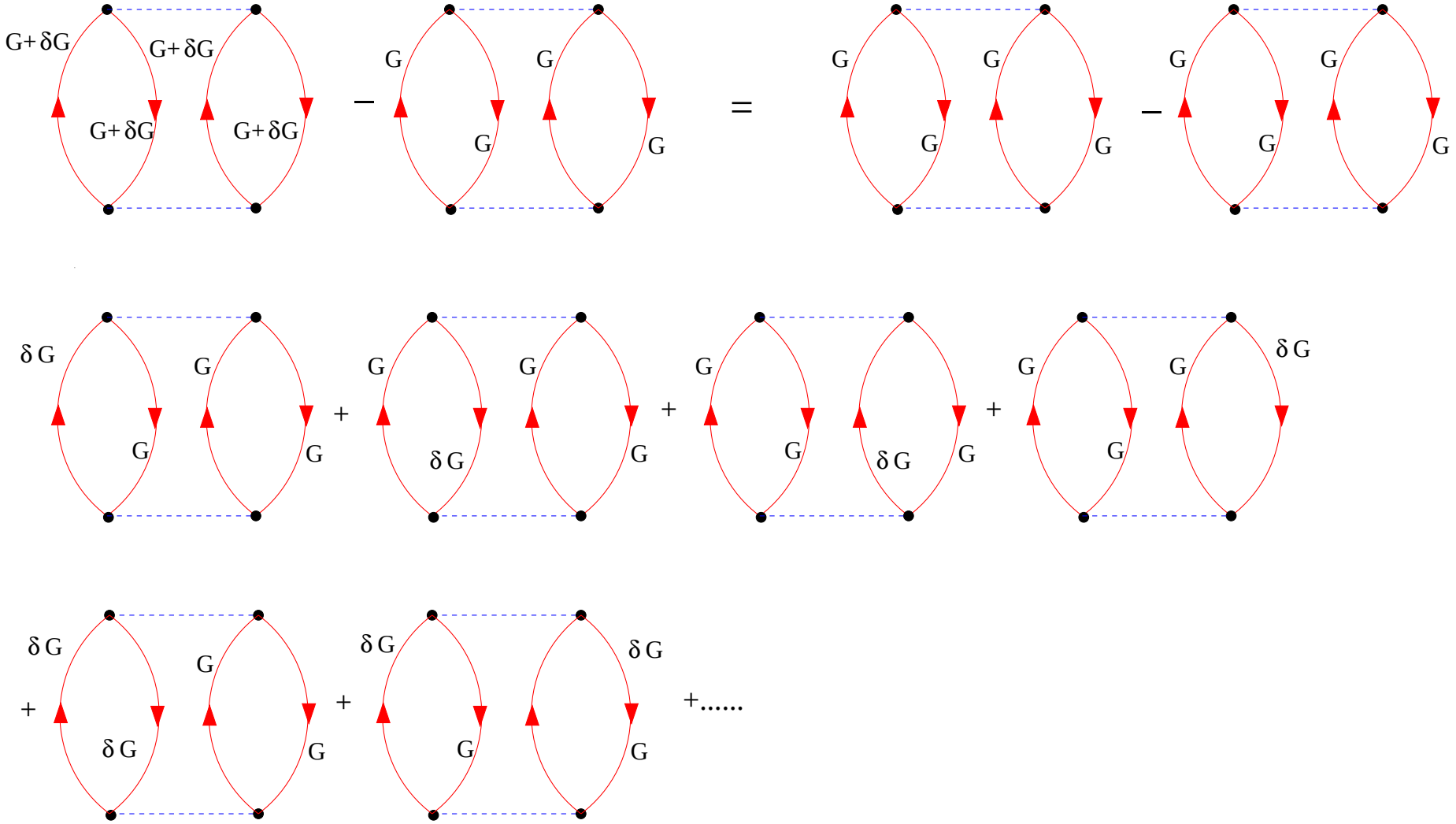
What is the meaning of the 'substituted' diagrams?



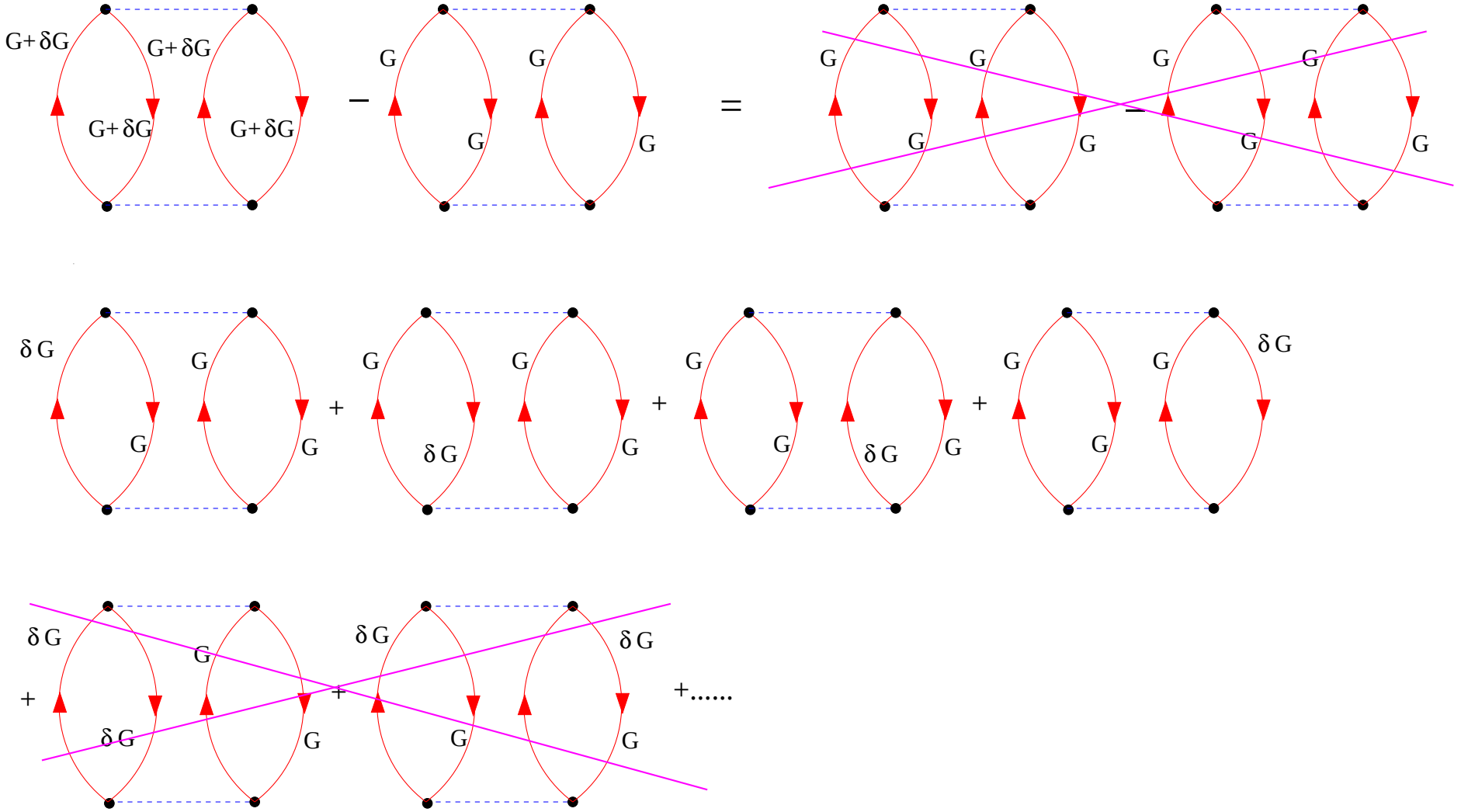

$$\left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma,\delta} \sum_{\alpha_1,\beta_1,\gamma_1,\delta_1} \sum_{\nu,\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k},\mathbf{k}',\mathbf{q})\; V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{q},-\mathbf{q})$$

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

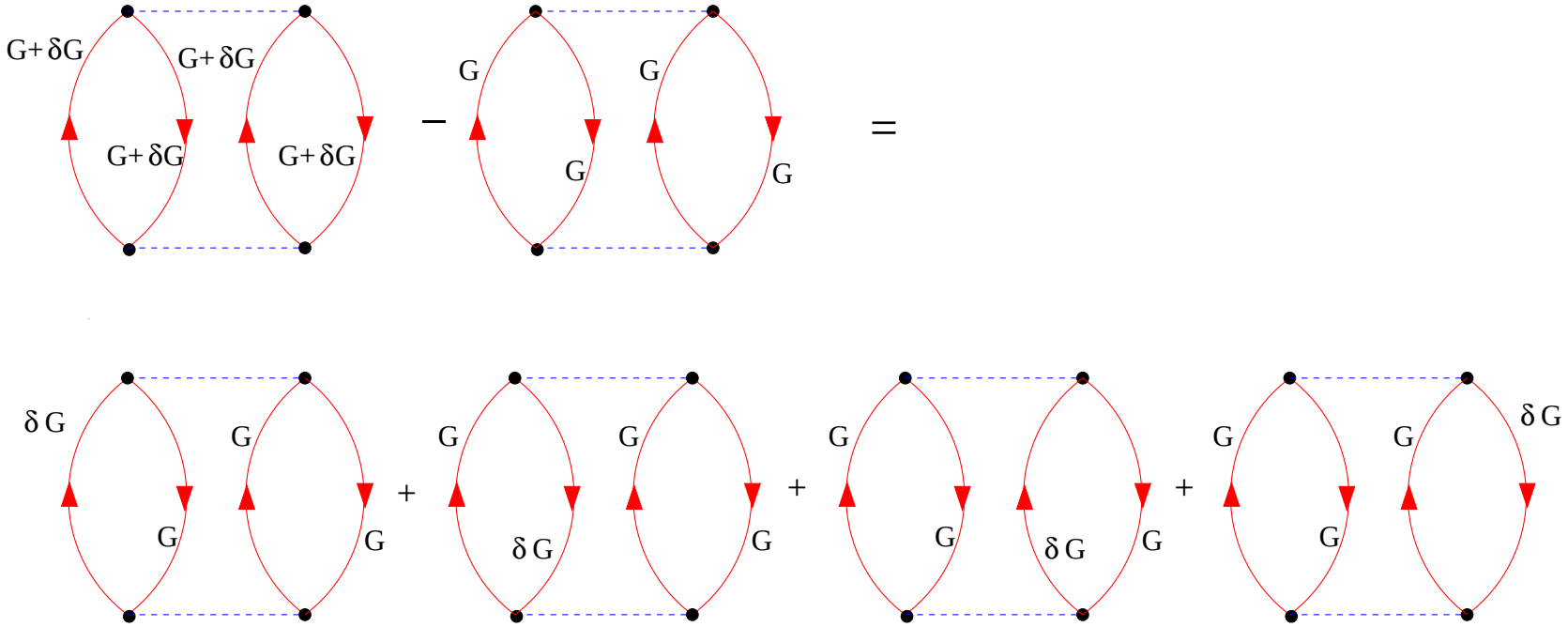
Let us consider the variation of $\Phi$ under a variation $G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) \rightarrow G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) + \delta G_{\alpha\beta}(\mathbf{k}, i\omega_\nu)$



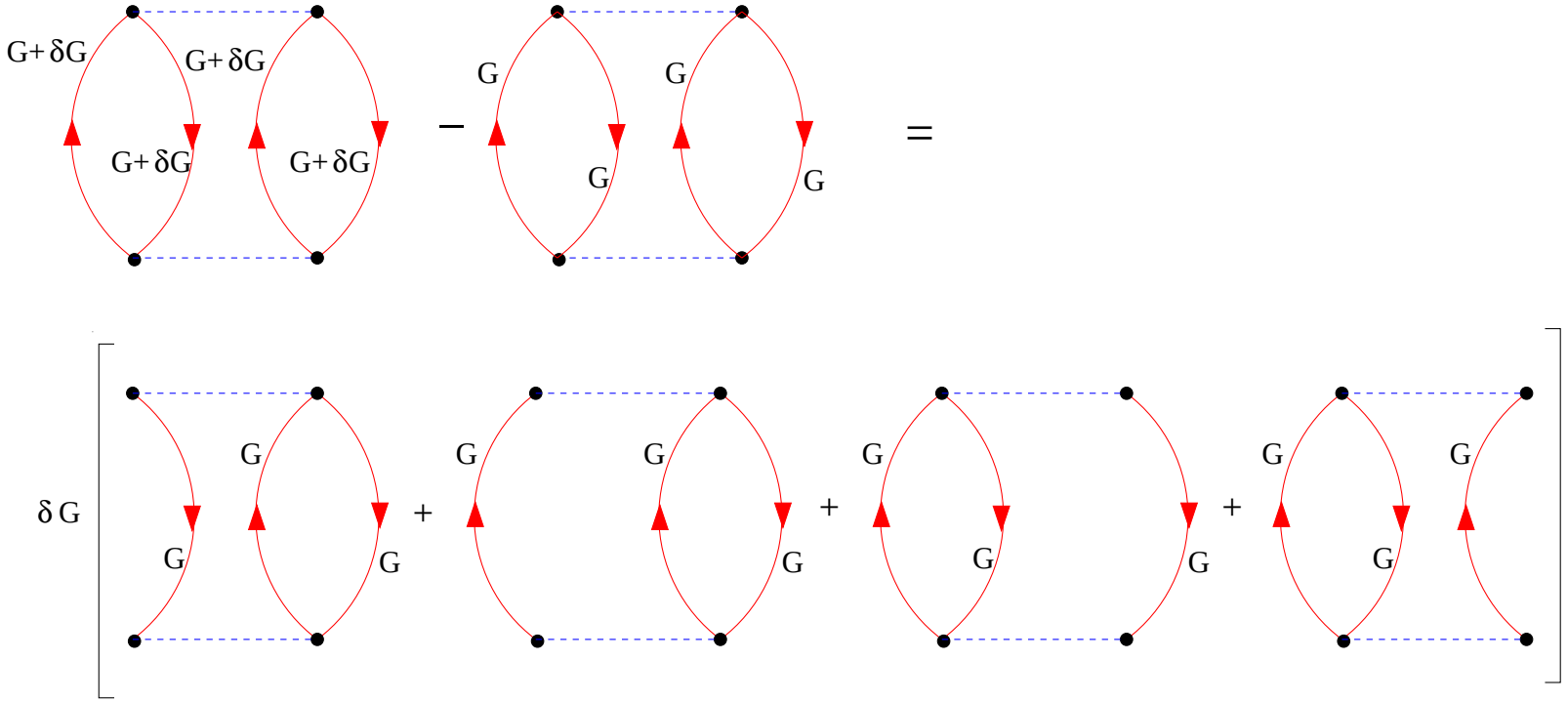
Let us consider the variation of $\Phi$ under a variation $G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) \rightarrow G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) + \delta G_{\alpha\beta}(\mathbf{k}, i\omega_\nu)$



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



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

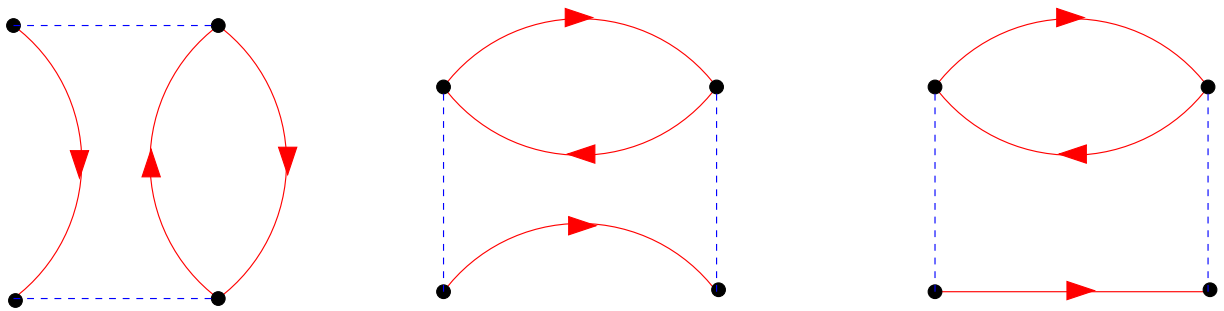


Forming the derivative

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

means 'opening' one of the Green's function lines in the diagrams contributing to $\Phi$

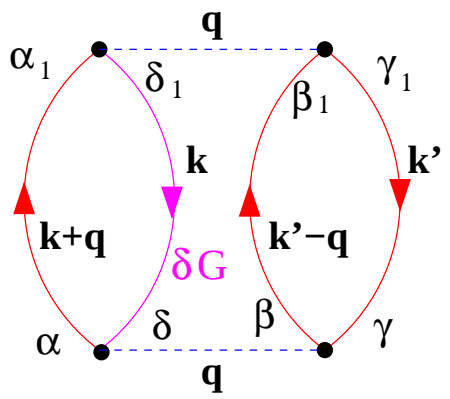
The 'opened' diagrams then indeed 'look like' self-energy diagrams:



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

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

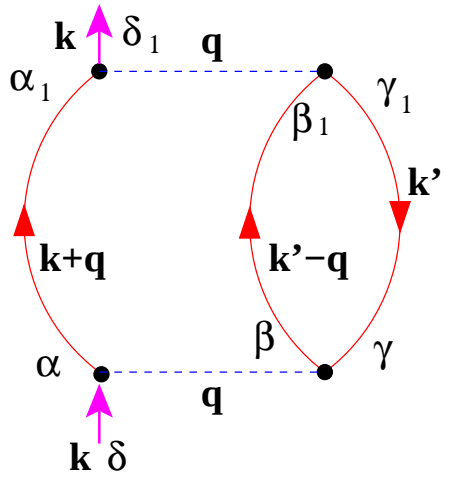
Factoring out the variation $\delta G$ 'fixes' the momentum, frequency and band indices of the remaining diagram




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

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

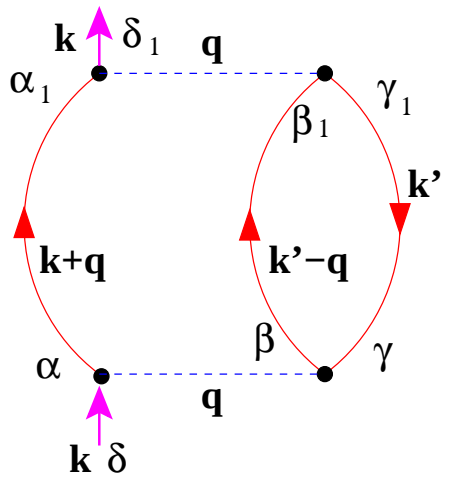
Factoring out the variation $\delta G$ 'fixes' the momentum, frequency and band indices of the remaining diagram




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

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

Factoring out the variation $\delta G$ 'fixes' the momentum, frequency and band indices of the remaining diagram

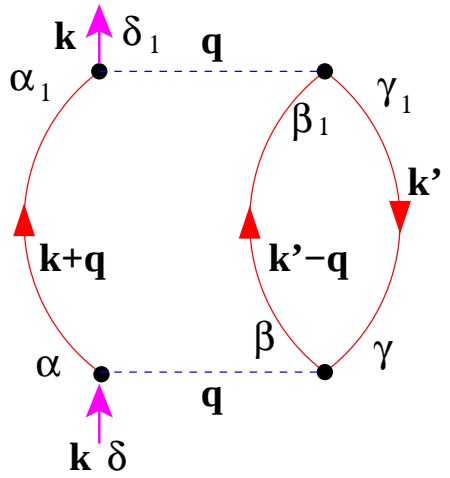



$$\delta G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu) \left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma} \sum_{\alpha_1,\beta_1,\gamma_1} \sum_{\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k}, \mathbf{k}', \mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},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

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

- The incoming and outgoing momentum and frequency are $\mathbf{k}$ and $\omega_\nu$
- 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 $\delta G$ 'fixes' the momentum, frequency and band indices of the remaining diagram

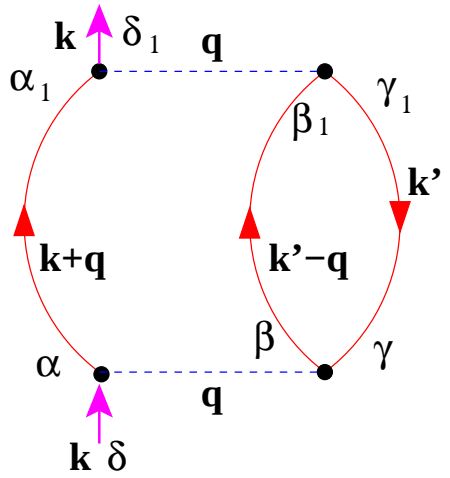



$$\delta G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu) \left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma} \sum_{\alpha_1,\beta_1,\gamma_1} \sum_{\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k}, \mathbf{k}', \mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},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

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

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

Factoring out the variation $\delta G$ 'fixes' the momentum, frequency and band indices of the remaining diagram



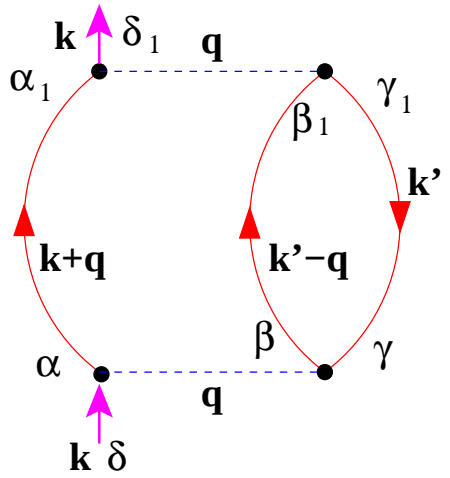

$$\delta G_{\delta,\delta_1}(\mathbf{k}, i\omega_\nu) \left(\frac{-1}{\beta\hbar^2 N}\right)^2 (-1)^2 \sum_{\mathbf{k}',\mathbf{q}} \sum_{\alpha,\beta,\gamma} \sum_{\alpha_1,\beta_1,\gamma_1} \sum_{\nu',\mu} V_{\alpha,\beta,\delta,\gamma}(\mathbf{k}, \mathbf{k}', \mathbf{q})\, V_{\delta_1,\gamma_1,\alpha_1,\beta_1}(\mathbf{k}+\mathbf{q},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

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

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

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

Factoring out the variation $\delta G$ 'fixes' the momentum, frequency and band indices of the remaining diagram




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

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

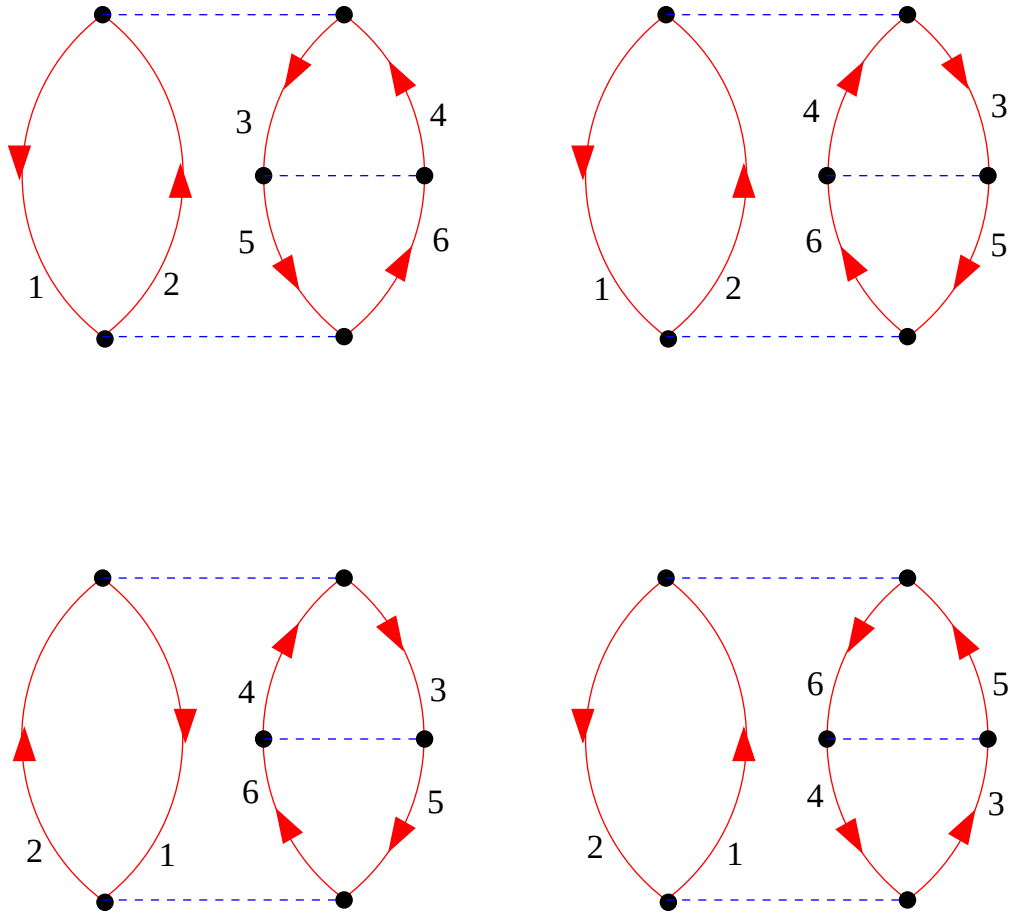
- Opening one Green's function lines reduces the number of Fermion loops $F$ by $1 \rightarrow$ the factor $(-1)^F$ changes sign - the extra (-1) in the prefactor takes care of this:

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

What about the factor $1/S$?

- Let us consider an $n^{th}$ order $\Phi$-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 $\Phi$-diagram gives $2n/S$ $\Sigma$-diagrams and each is produced $S$ times
- This factor of $S$ exactly cancels the factor of $1/S$ in the prefactor of the diagram

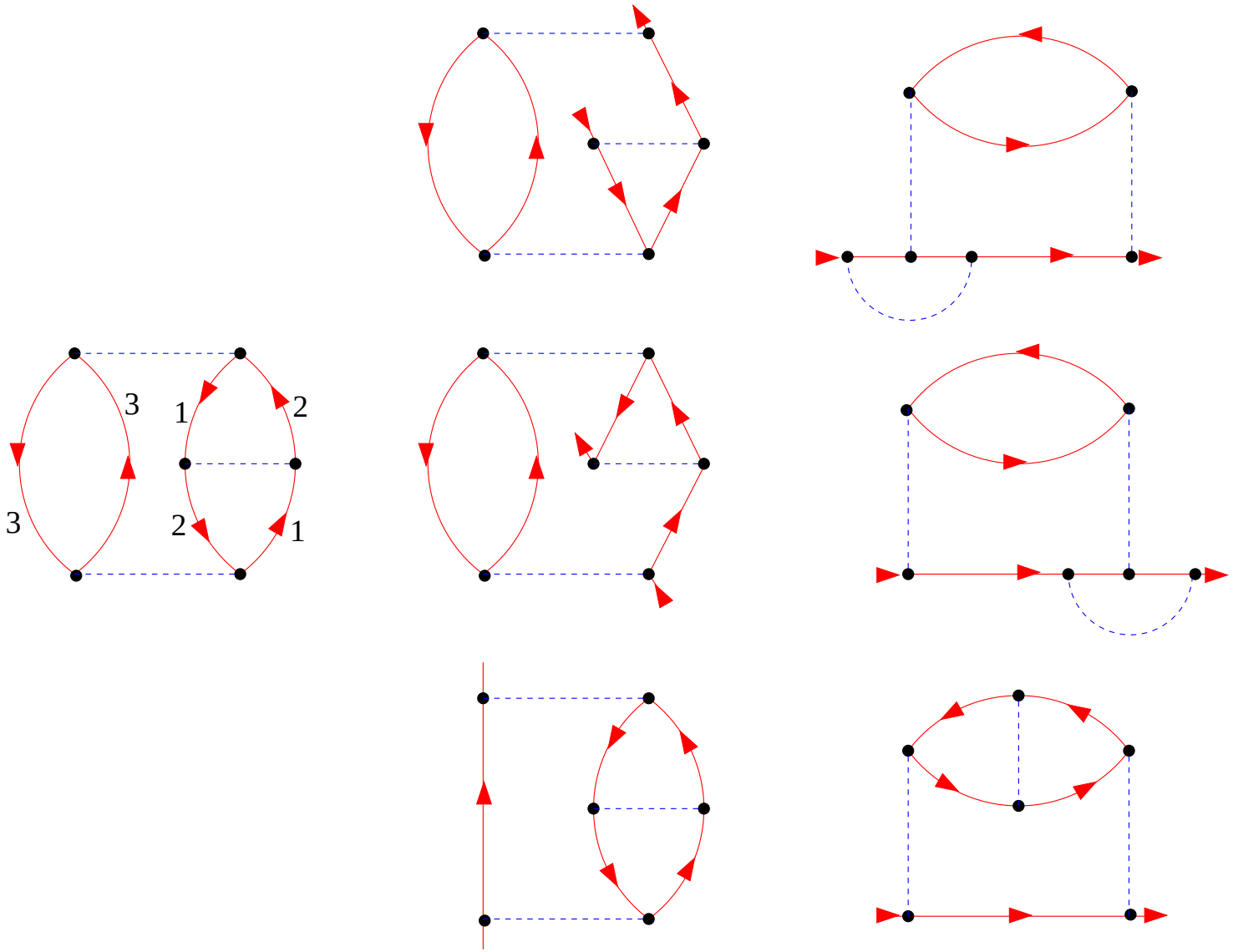
## Example



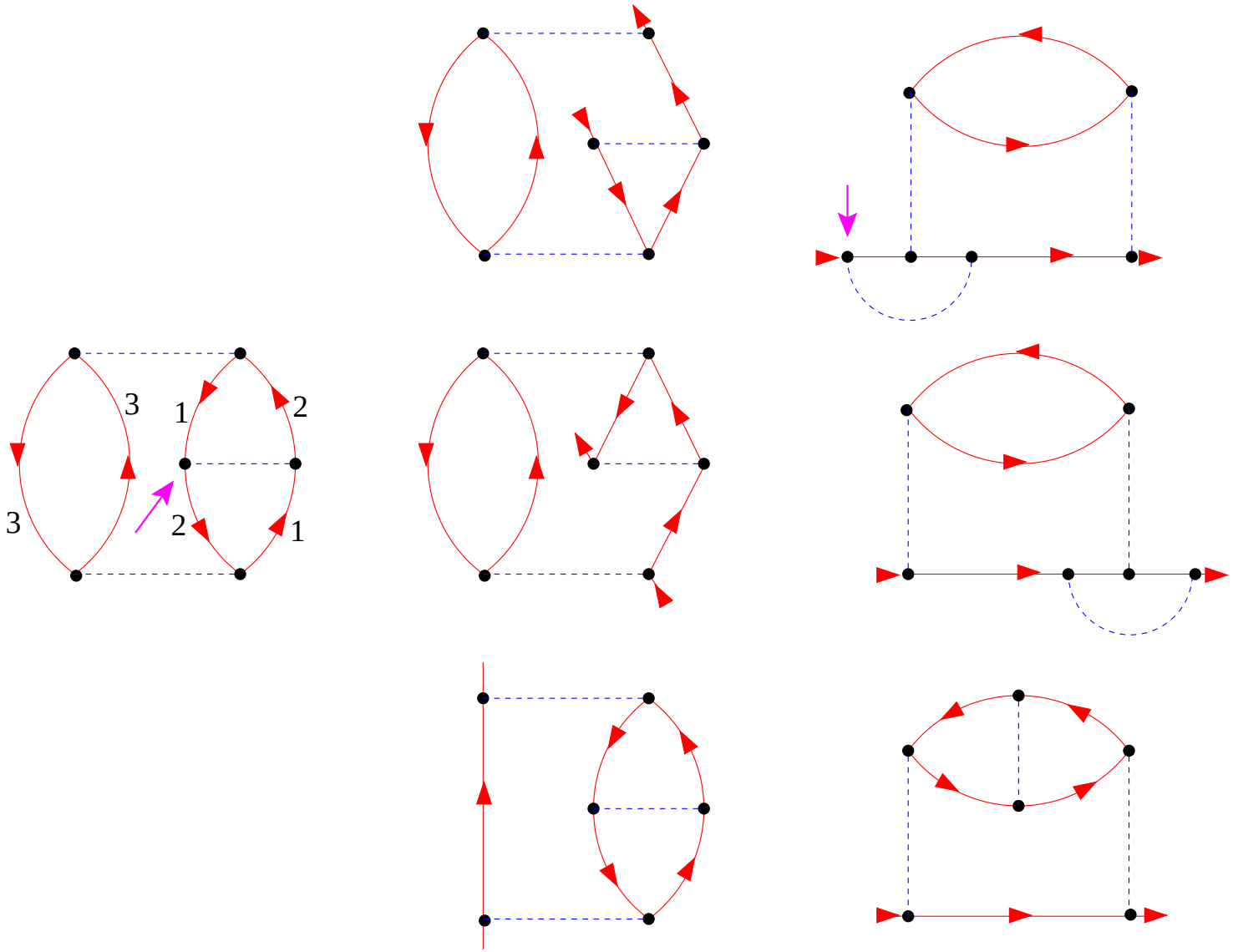

For this diagram there are no further symmetry operations $\rightarrow$ the diagram has $S = 2$ (we include identity!)

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

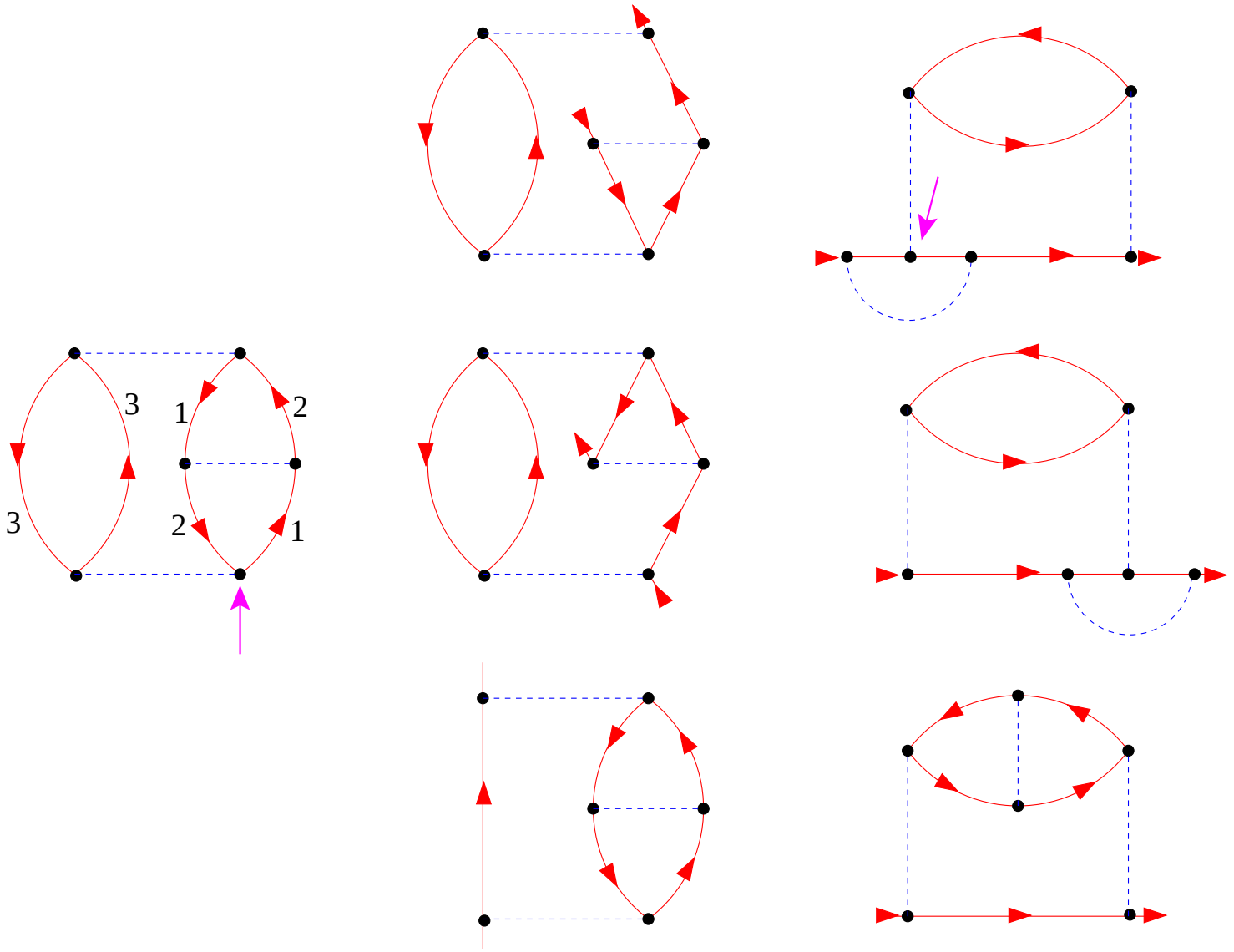
# Example, cont'd



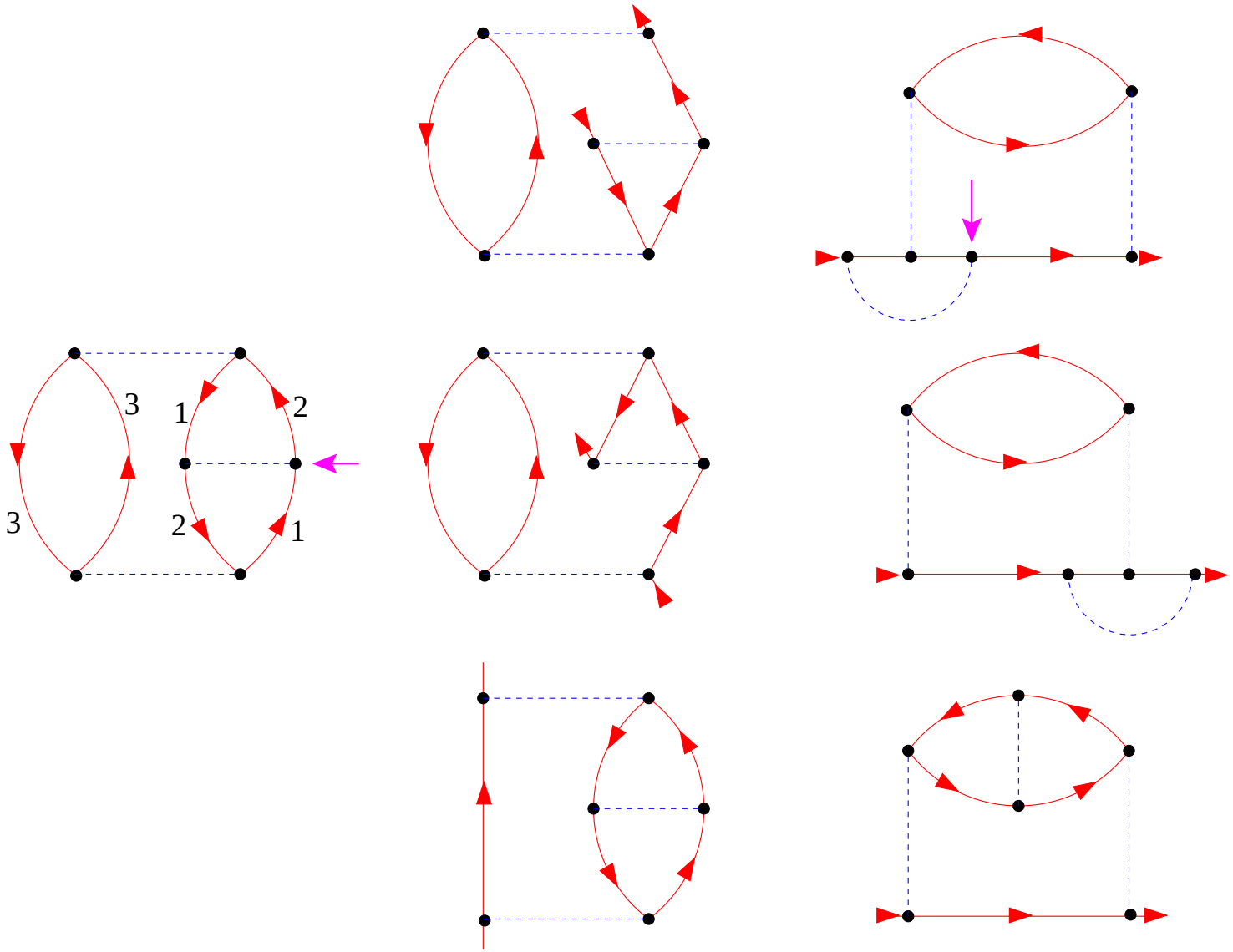
# Example, cont'd



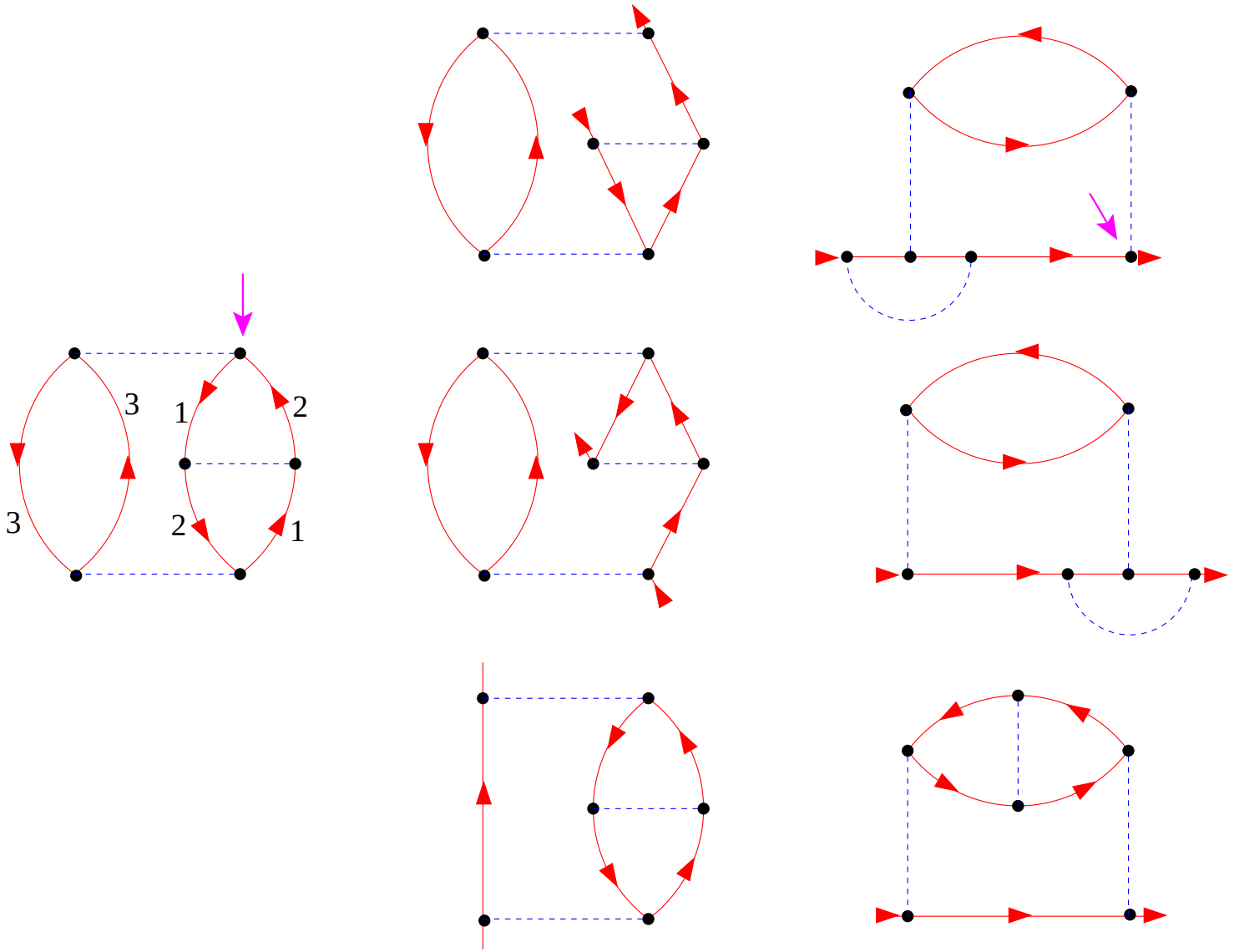
# Example, cont'd



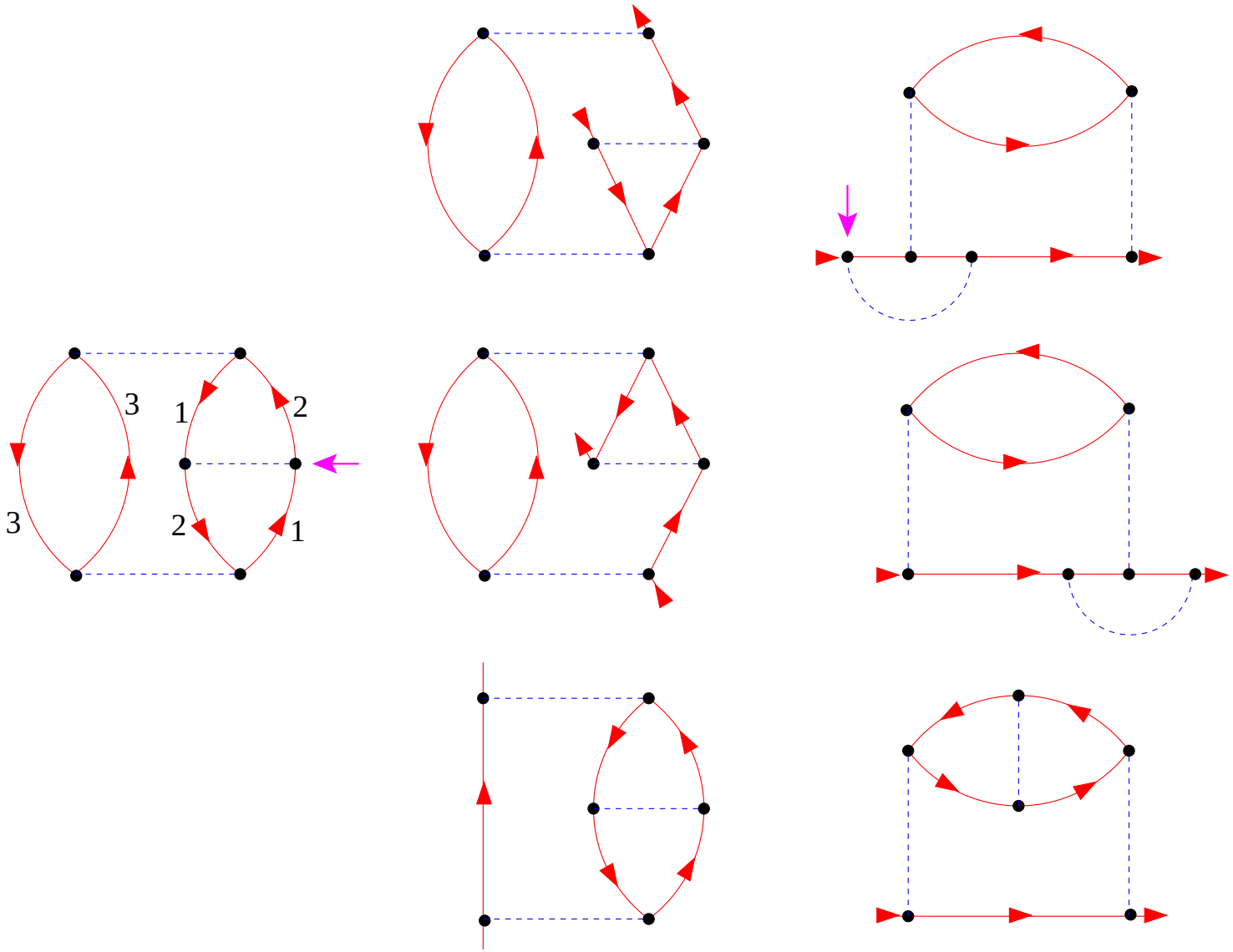
# Example, cont'd



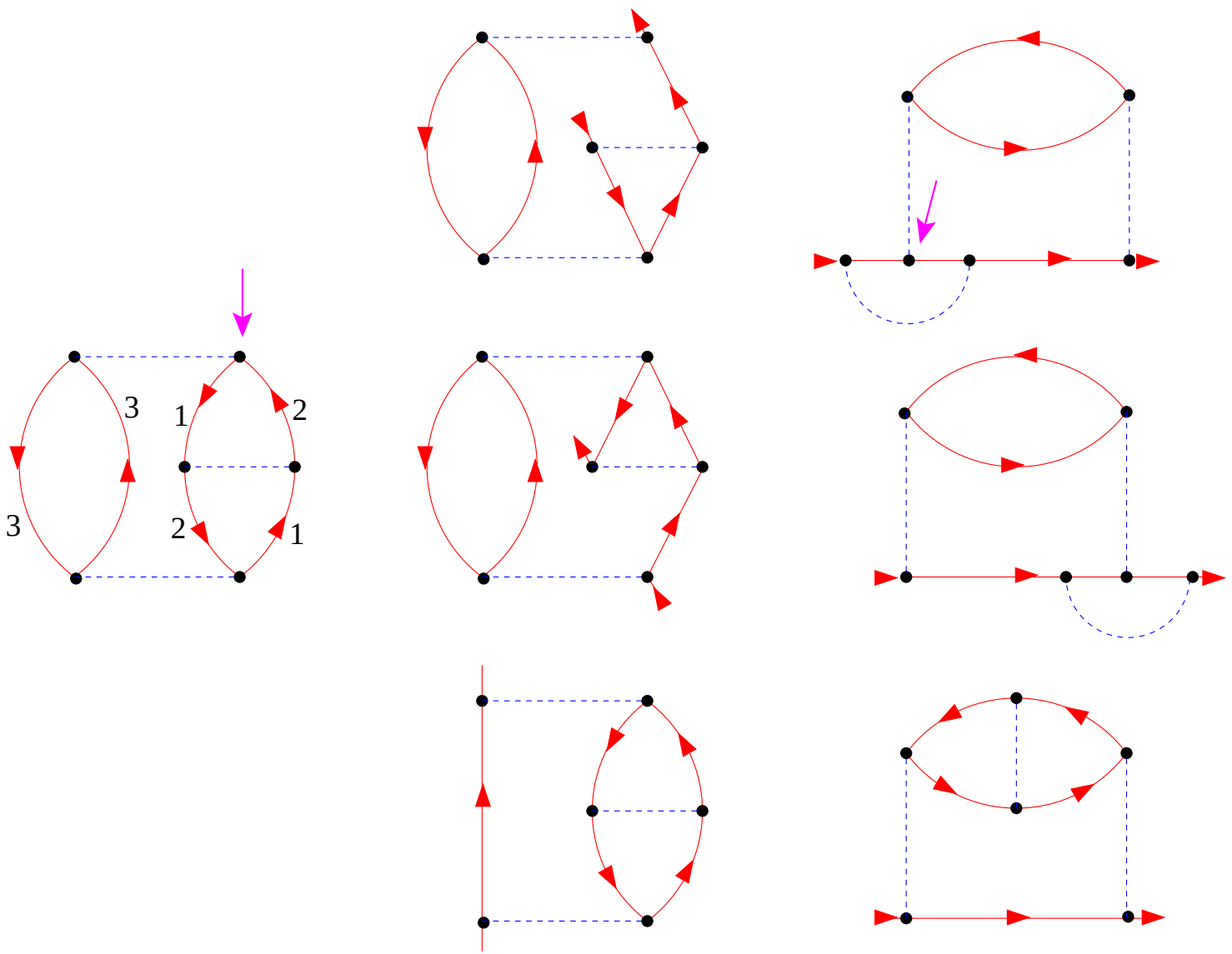
# Example, cont'd



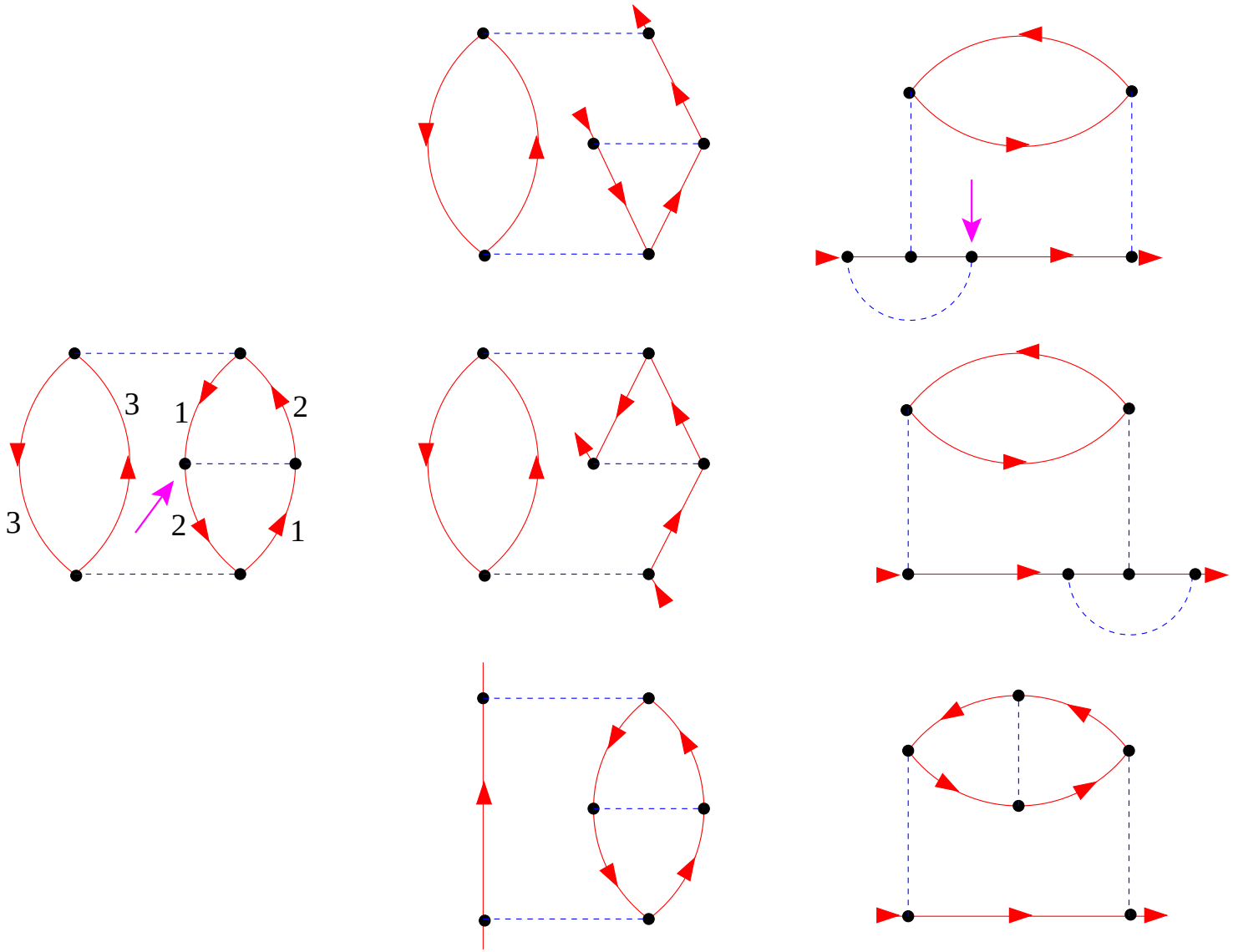
# Example, cont'd



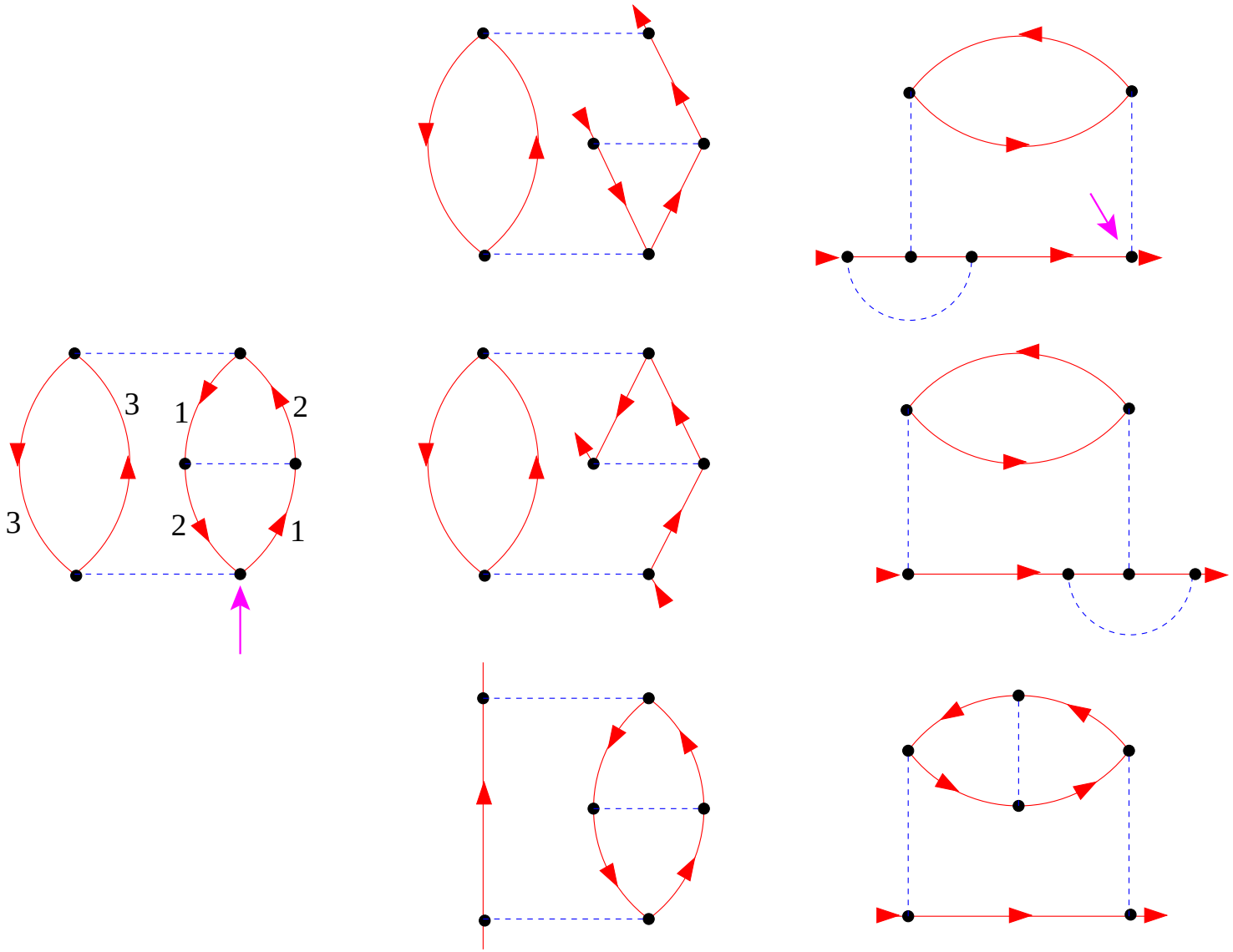
# Example, cont'd



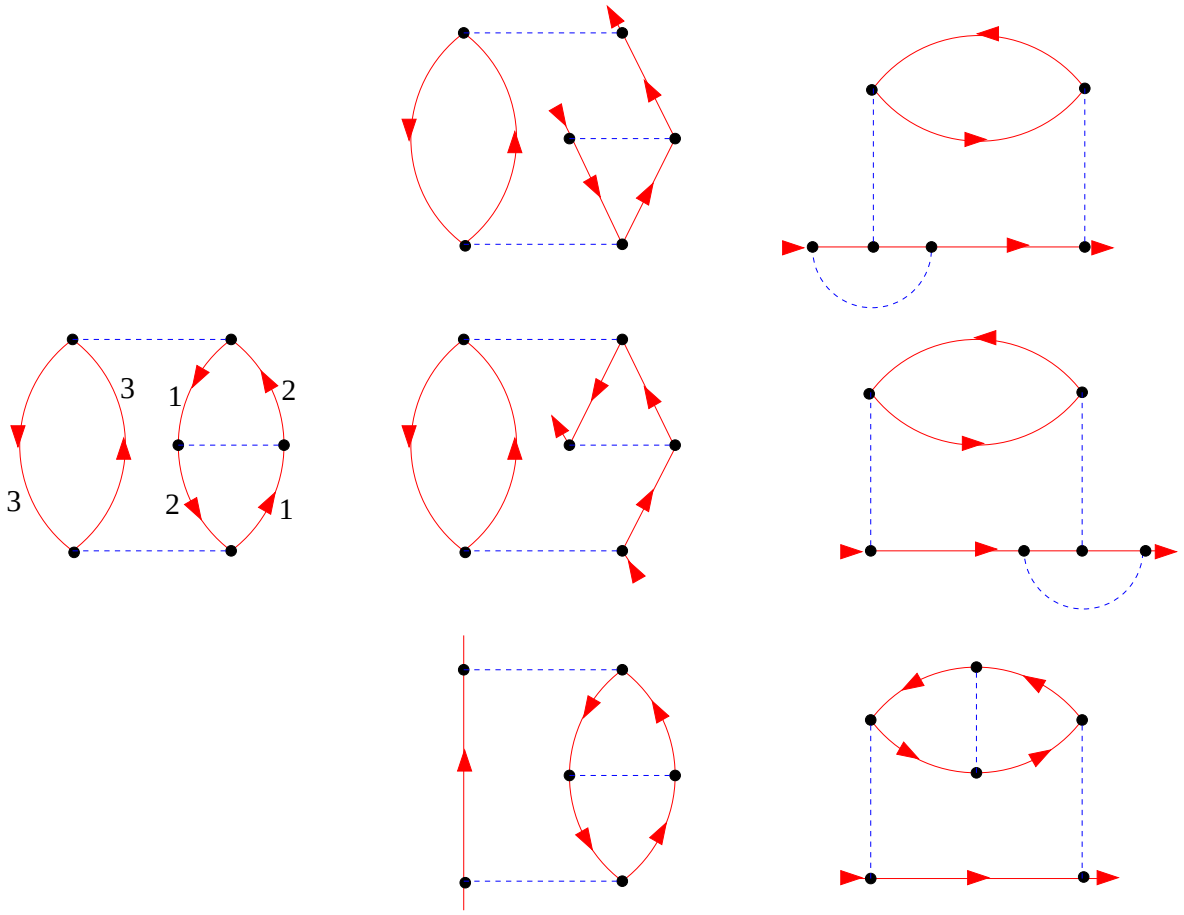
# Example, cont'd



# Example, cont'd



## Example, cont'd




- The diagram has $n = 3$ and $S = 2 \longrightarrow 3$ 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

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

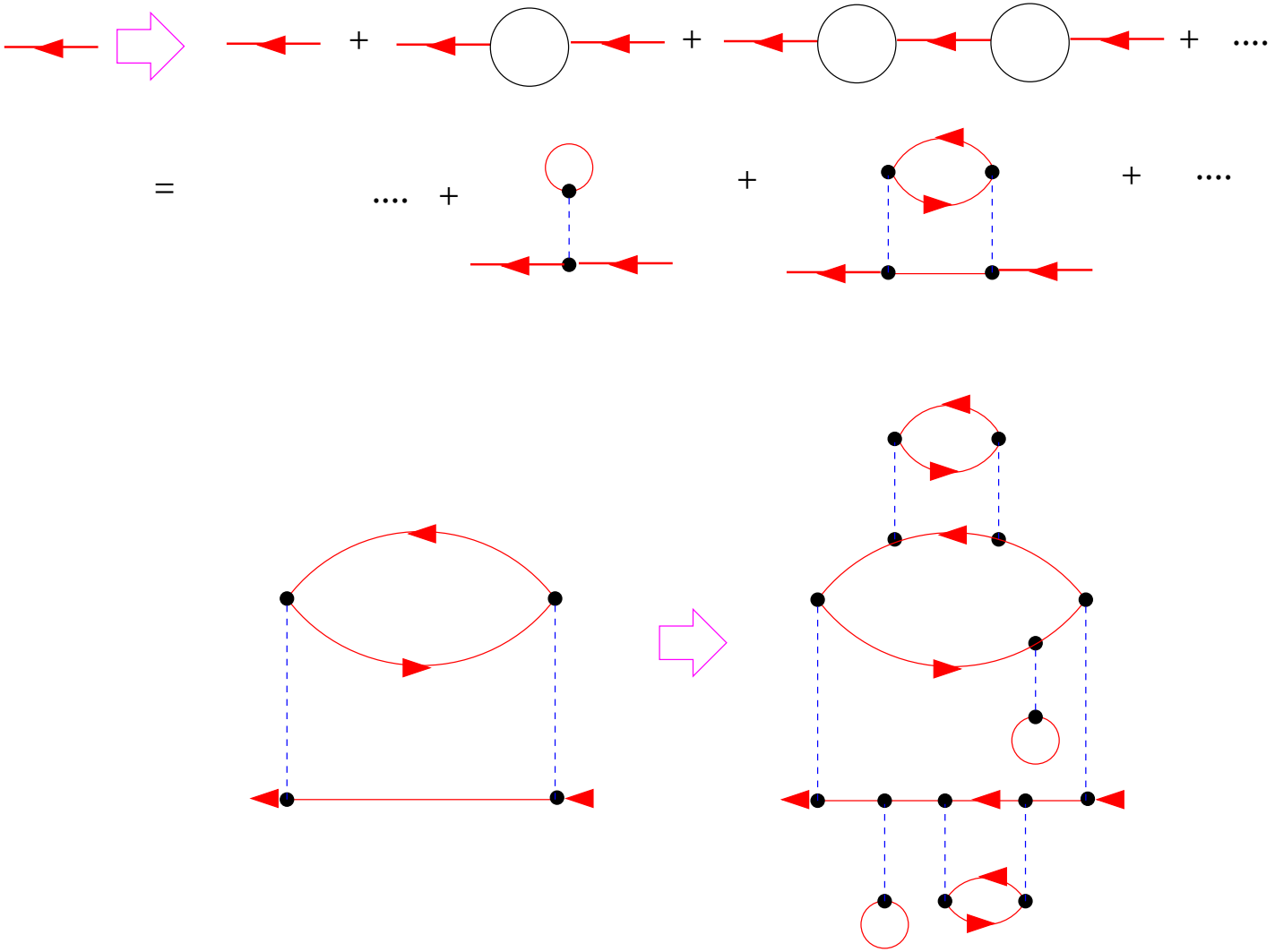
gives precisely all skeleton diagrams for $\Sigma_{\beta,\alpha}(\mathbf{k}, i\omega_\nu)$ but with the the Green's function $\mathbf{G}$ used for all Green's function lines (and a prefactor $1/\beta$)

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

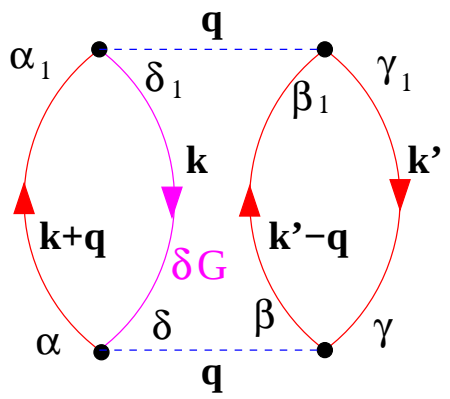
$$\frac{\partial \Phi[\mathbf{G}]}{\partial G_{\alpha,\beta}(\mathbf{k}, i\omega_\nu)} = \frac{1}{\beta} \Sigma_{\beta,\alpha}(\mathbf{k}, i\omega_\nu)$$

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?

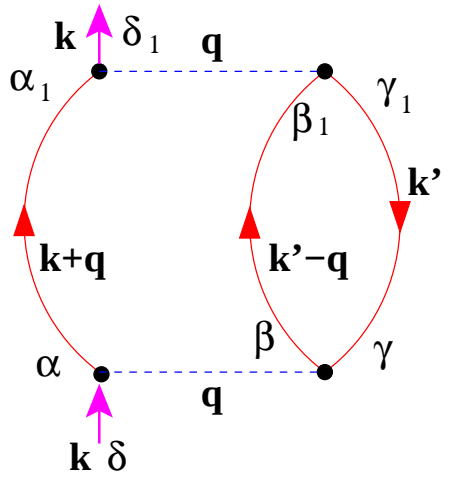
Factoring out the variation $\delta G$ 'fixes' the momentum, frequency and band indices of the remaining diagram




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

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

Factoring out the variation $\delta G$ '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

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

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

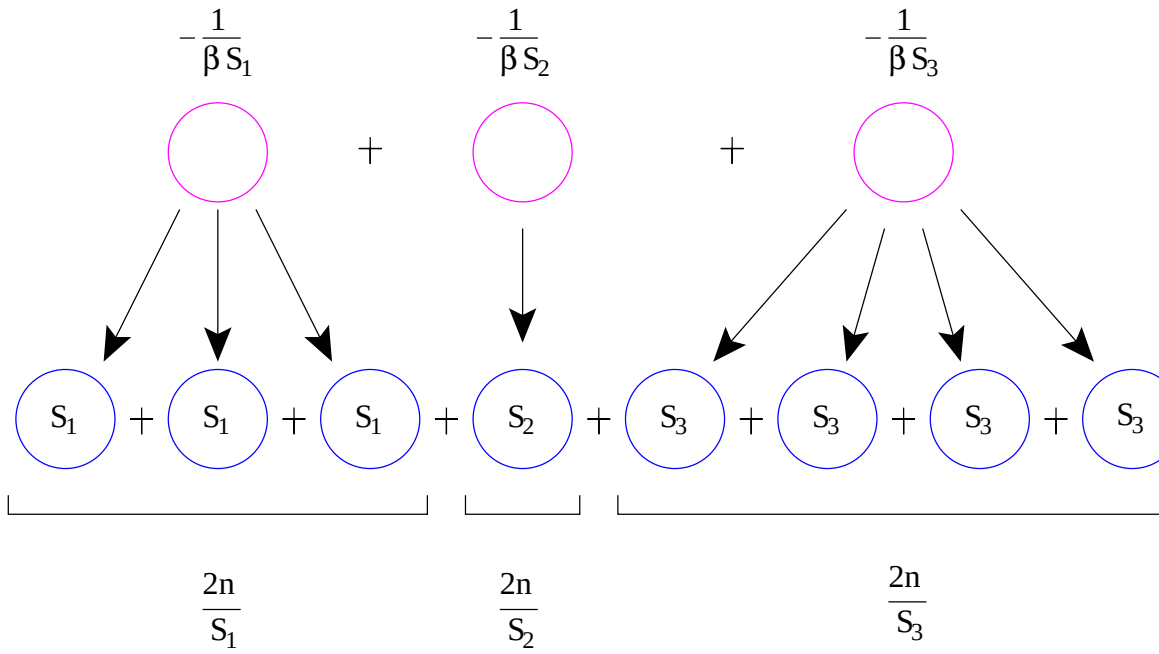
$\Phi^{(n)}$ is the sum of all $n^{th}$ order diagrams for $\Phi$: closed, linked skeleton diagrams, with Green's function lines standing for the full Green's function $\mathbf{G}$

$\boldsymbol{\Sigma}^{(s,n)}_{\beta,\alpha}(\mathbf{k},i\omega_\nu)$ 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 $\boldsymbol{\Sigma}$ because we only want skeleton diagrams for $\Phi$

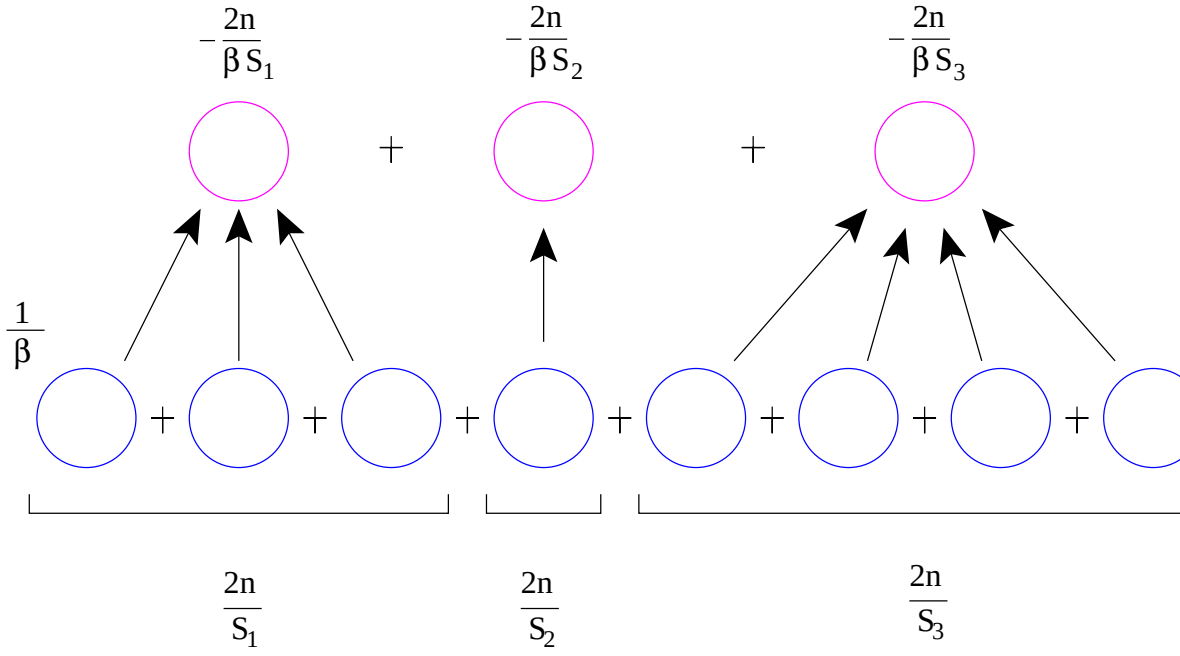
However, again we need to be careful about prefactors!

We consider $n^{th}$-order diagrams for $\Phi$ and $\Sigma$




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'

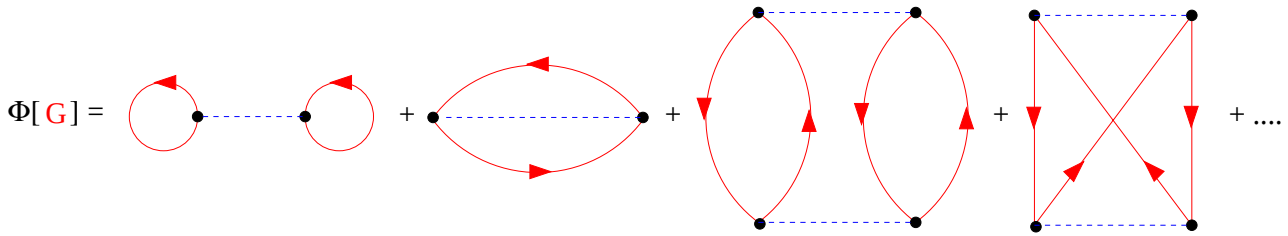
## Calculation of $\lambda \frac{\partial \Omega'}{\partial \lambda}$

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

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 $\lambda$!)




We treat these two variations separately and first consider the variation of $\Omega'$ 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)

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

then becomes

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

- 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 $\Sigma$ 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

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

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

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 $\Phi$ is the generating functional of $\Sigma$

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

Then we have

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

$\Omega'$ 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

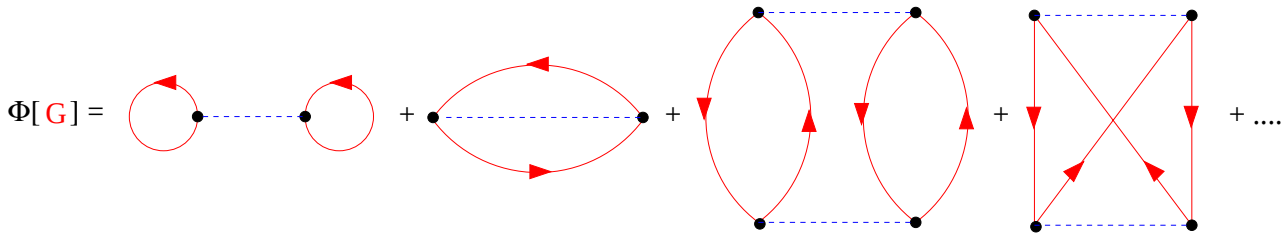
## Calculation of $\lambda \frac{\partial \Omega'}{\partial \lambda}$

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

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 $\Omega'$ is zero!
- The interaction lines in the Luttinger-Ward functional will change

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




Accordingly we study the change of $\Phi$ under a change of $\lambda$ (prefactor of all interaction lines) when $\Sigma$ 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 $\lambda^n$

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)

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

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

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

- $\Omega$ is stationary with respect to variations of the self-energy

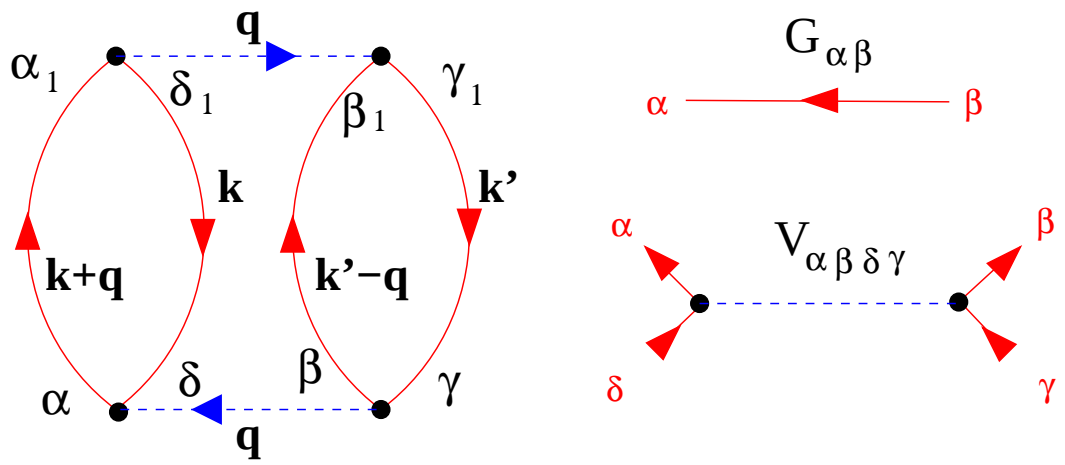
$$\frac{\partial\Omega}{\partial\Sigma_{\alpha\beta}(\mathbf{k},i\omega_\nu)}=0$$

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

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

- The Luttinger-Ward functional is a sum over infinitely many Feynman diagrams - hard to evaluate....
- The Luttinger-Ward functional involves only the matrix elements of $H_1$ and is independent of the noninteracting part of the Hamiltonian Hamiltonian $H_0$
- This implies in particular that two systems with the same $H_1$ but different $H_0$ have the same Luttinger-Ward functional $\Phi[G]$ - this will be of major importance in a moment!

The properties of the system under study enter only at one point




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

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

The only property of the system which enters the functional $\Phi$ therefore are the interactions lines - that means the matrix elements of the interaction

This implies in particular that the elements of the single-particle Hamiltonian $H_0$ appear nowhere in the Luttinger-Ward functional

## Summary of the Proof

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

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

- $\Omega$ 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

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

- The Luttinger-Ward functional is a sum over infinitely many Feynman diagrams - hard to evaluate....
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- This implies in particular that two systems with the same $H_1$ but different $H_0$ have the same Luttinger-Ward functional $\Phi[G]$ - this will be of major importance in a moment!

## Some remarks

- The theorem is the basis for various important developments in field theory: the Luttinger theorem and the 'conserving approximations' (GW, FLEX)
- The proof above assumes a continouous evolution of the system as $H_1$ is switched on - which is highly questionable in a correlated insulator....
- However, Potthoff has recently given a non-perturbative proof of the existence of a functional with all properties listed above (reference in the notes)

## The Legendre transform of the Luttinger-Ward functional

Reminder:

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

Now define the Legendre transform

$$\begin{aligned} F[\mathbf{\Sigma}] &= \Phi[\mathbf{G}[\mathbf{\Sigma}]] - \sum_{\mathbf{k},\nu} \sum_{\alpha,\beta} \frac{\partial \Phi}{\partial G_{\alpha\beta}(\mathbf{k}, i\omega_\nu)}\; G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) \\ &= \Phi[\mathbf{G}[\mathbf{\Sigma}]] - \frac{1}{\beta} \sum_{\mathbf{k},\nu} \sum_{\alpha,\beta} \Sigma_{\beta\alpha}(\mathbf{k}, i\omega_\nu)\; G_{\alpha\beta}(\mathbf{k}, i\omega_\nu) \\ &= \Phi[\mathbf{G}[\mathbf{\Sigma}]] - \frac{1}{\beta} \sum_{\mathbf{k},\nu} \text{trace}\; \mathbf{G}(\mathbf{k}, i\omega_\nu)\; \mathbf{\Sigma}(\mathbf{k}, i\omega_\nu). \end{aligned}$$

We had

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

We had

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

$$= -\lim_{\eta\to 0^+} \frac{1}{\beta} \sum_{\mathbf{k},\nu} e^{i\omega_\nu \eta} \left[ \ln \det \left( -i\omega_\nu + \frac{1}{\hbar}\left(\mathbf{t}(\mathbf{k}) - \mu\right) + \boldsymbol{\Sigma}(\mathbf{k}, i\omega_\nu \right) \right] + F\left[\boldsymbol{\Sigma}\right]$$

In this way we have expressed $\Omega$ as a functional of $\boldsymbol{\Sigma}$ which is stationary at the exact $\boldsymbol{\Sigma}$:

$$\frac{\delta\Omega}{\delta\boldsymbol{\Sigma}} = 0$$

We could now try to derive the Euler-Lagrange equation for $\boldsymbol{\Sigma}$ (i.e. the analogue of the Kohn-Sham equations in DFT) or use a 'trial $\boldsymbol{\Sigma}$' with a number of variational parameters

$$\Sigma(\omega) = \eta + \sum_i \frac{\sigma_i}{\omega - \zeta_i}$$

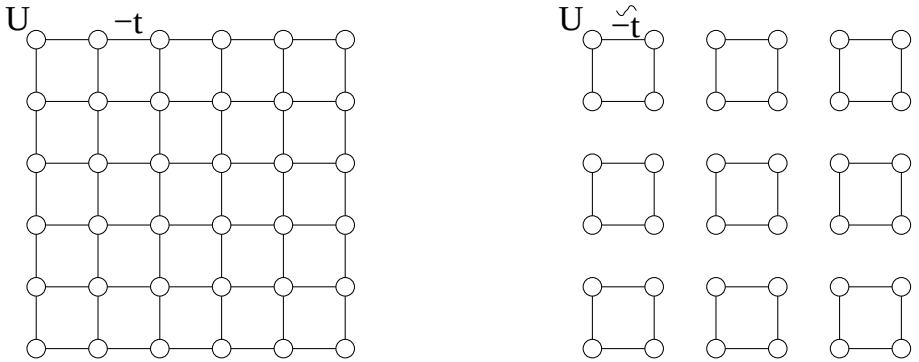
The problem: We do not know the functional $F\left[\boldsymbol{\Sigma}\right]$

## Basic Idea of the VCA

Let us assume that we are interested in the 2D Hubbard model on an infinite square lattice

$$H = \sum_{i,j} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

We partition the square lattice into finite clusters - say $2 \times 2$




The Hamiltonian for the $2 \times 2$ clusters is

$$\tilde{H} = \sum_{\{i,j\} \in Cluster} \tilde{t}_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

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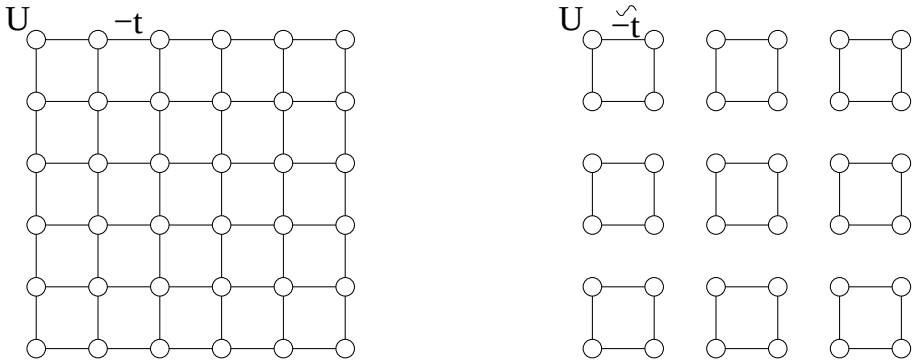



The Hamiltonian for the $2 \times 2$ clusters is

$$\tilde{H} = \sum_{\{i,j\} \in Cluster} \tilde{t}_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Both systems have the same interaction part $\longrightarrow$ they have the same Luttinger-Ward functional

- The $2 \times 2$ clusters can be solved exactly by exact diagonalization
- This means all eigenstates $|i\rangle$ and their energies $E_i$ and particle number $N_i$ are known
- We can therefore evaluate the Grand Partition Function $\tilde{Z}$ and $\tilde{\Omega} = -k_B\, T\, log(\tilde{Z})$

$$\tilde{Z} \;=\; \sum_i \; e^{-\beta(E_i - \mu N_i)}$$

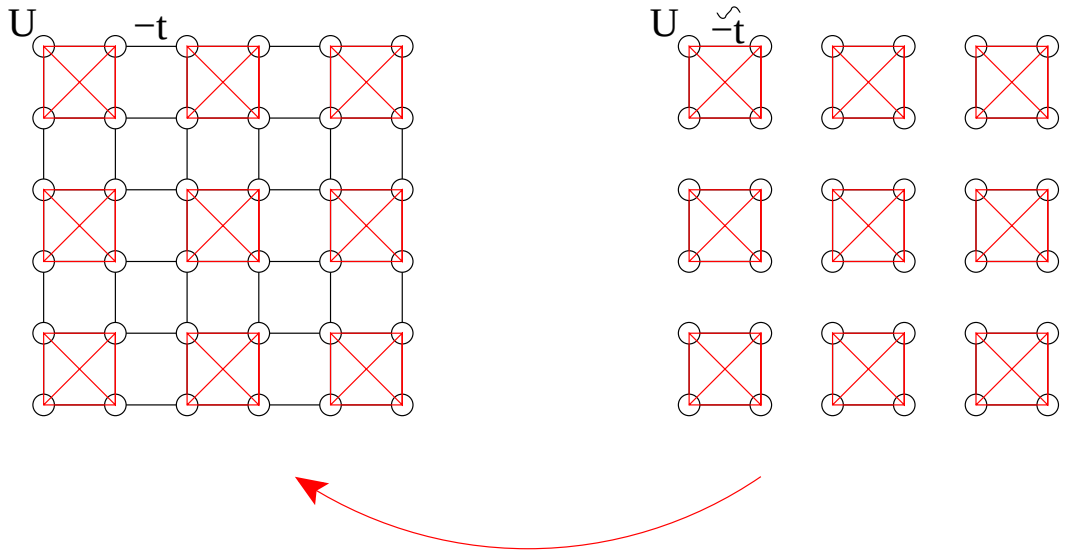
(it is actually sufficient to know all eigenstates with $E - \mu N$ within $\approx 10 k_B T$ above the GS so that rather large clusters can be treated by Lanczos)

- Moreover we can evaluate the Green's function $\tilde{G}_{ij}(\omega)$ $(i, j \in \{1, 4\})$
- For given $\omega$ we can invert the matrix $\tilde{G}_{ij}(\omega)$ numerically and obtain $\tilde{\Sigma}_{ij}(\omega)$ from the Dyson equation
- Now we can revert the Luttinger-Ward expression for $\tilde{\Omega}$ and obtain the numerical value of $F[\tilde{\Sigma}]$

$$F[\tilde{\mathbf{\Sigma}}] \;=\; \tilde{\Omega} + \lim_{\eta \to 0^+} \; \frac{1}{\beta} \sum_\nu \; e^{i\omega_\nu \eta} \; \left[ \ln \; \det \left( -\omega - \frac{1}{\hbar}\, \mu + \frac{1}{\hbar}\, \tilde{\mathbf{t}} + \tilde{\mathbf{\Sigma}}(i\omega_\nu) \right) \right]$$

This gives us the self-energy $\tilde{\mathbf{\Sigma}}(\omega)$ and the numerical value of its Luttinger-Ward functional $F[\tilde{\mathbf{\Sigma}}]$

Now we use the self-energy $\tilde{\mathbf{\Sigma}}(\omega)$ as a trial self-energy for the infinite system




$$\mathbf{G}'(\mathbf{k},\omega) \;=\; \left(\omega + \frac{1}{\hbar}\,\mu - \frac{1}{\hbar}\,\mathbf{t}(\mathbf{k}) - \tilde{\mathbf{\Sigma}}(\mathbf{k},\omega)\right)^{-1}$$

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

(Note: this will obviously introduce an artificial supercell structure into the infinite system)

How do we perform a variation of the self-energy?

$$\mathbf{G}'(\mathbf{k},\omega) \;=\; \left(\omega + \frac{1}{\hbar}\,\mu - \frac{1}{\hbar}\,\mathbf{t}(\mathbf{k}) - \tilde{\mathbf{\Sigma}}(\mathbf{k},\omega)\right)^{-1}$$

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

Reminder: the Hamiltonian of the cluster was

$$\tilde{H} \;=\; \sum_{\{i,j\}\in Cluster} \tilde{t}_{ij}\; c^\dagger_{i\sigma}c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

The only requirement on $\tilde{H}$ was that the interaction part is the same as the lattice system

There is nothing that fixes the the single-particle matrix elements $\tilde{t}_{ij}$

On the other hand changing the $\tilde{t}_{ij}$ will change $\tilde{\mathbf{\Sigma}}(\omega)$ and therefore $\Omega_{latt}$: $\Omega_{latt} = \Omega_{latt}(\tilde{t}_{ij})$

We therefore replace

$$\frac{\delta\Omega_{latt}}{\delta\Sigma} = 0 \;\rightarrow\; \frac{\partial\Omega_{latt}}{\partial\tilde{t}_{ij}} = 0$$

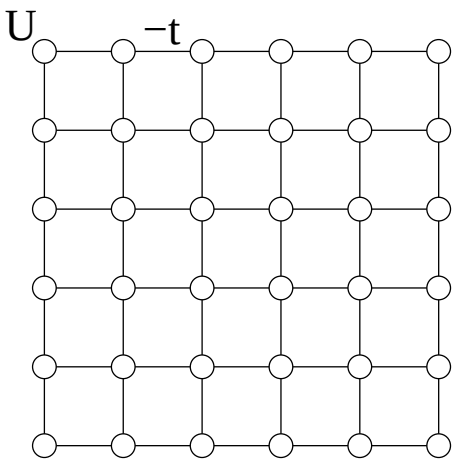
This is the basic idea of the VCA

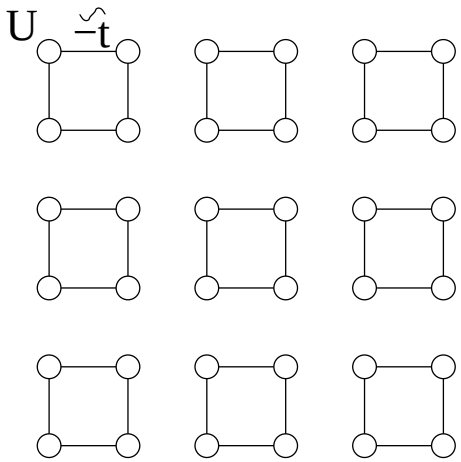
This means we are seeking the best approximation to the self-energy of the infinite lattice amongst 'cluster-representable' ones that means self-energies which can be generated as exact self-energies of a finite cluster

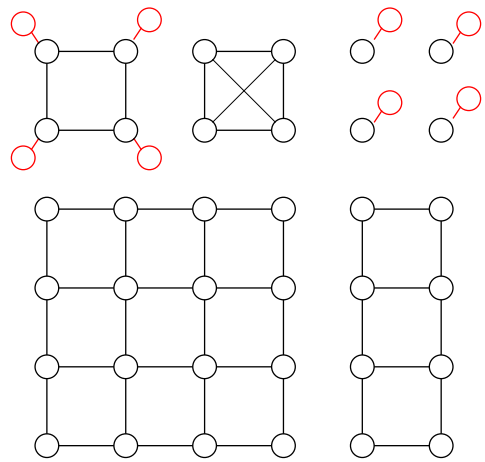
The problem that we do not know the functional form of $F[\Sigma]$ is bypassed by evaluating this numerically

## Remarks

- The system of clusters which is used to generate the 'trial self-energies' has been termed the reference system by Potthoff
- There is considerable freedom in choosing the reference system - for example one may include noninteracting 'bath sites'



- The problem with the artificial supercell can be solved: there is also a 'periodized' version of the VCA which is translationally invariant (W. Koller and N. Dupuis, J. Phys.: Condens. Matter **18** 9525 (2006))

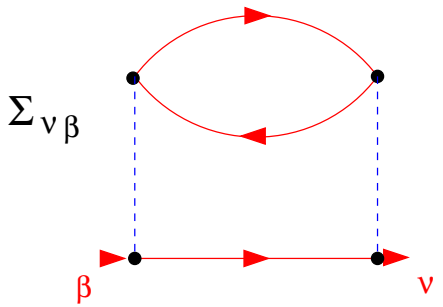
## Remark on 'bath' sites

A 'bath' site is an orbital $\rho$ without any interaction, i.e. the interaction term

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

does not contain any matrix element involving the orbital $\rho$

Obviously this implies that $\Sigma_{\rho,\alpha} = \Sigma_{\alpha,\rho} = 0$ for any $\alpha$: the self-energy has no matrix elements involving $\rho$



Example: Metal-Insulator Transition in a Dimer (M. Potthoff, Eur. Phys. J. B**36**, 335 (2003))

We consider a particle-hole symmetric Hubbard model (with $n_i = c^\dagger_{i\uparrow} c_{i\uparrow} + c^\dagger_{i\downarrow} c_{i\downarrow}$)

$$\begin{aligned} H - \mu N &= \sum_{i,j,\sigma} t_{ij}\, c^\dagger_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_{i=1}^{N} (n_i - 1)(n_i - 1) - N\, \frac{U}{2} \\ &= \sum_{i,j,\sigma} t_{ij}\, c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_{i=1}^{N} n_{i,\uparrow}\, n_{i,\downarrow} - \frac{U}{2} \sum_{i=1}^{N} n_i \end{aligned}$$

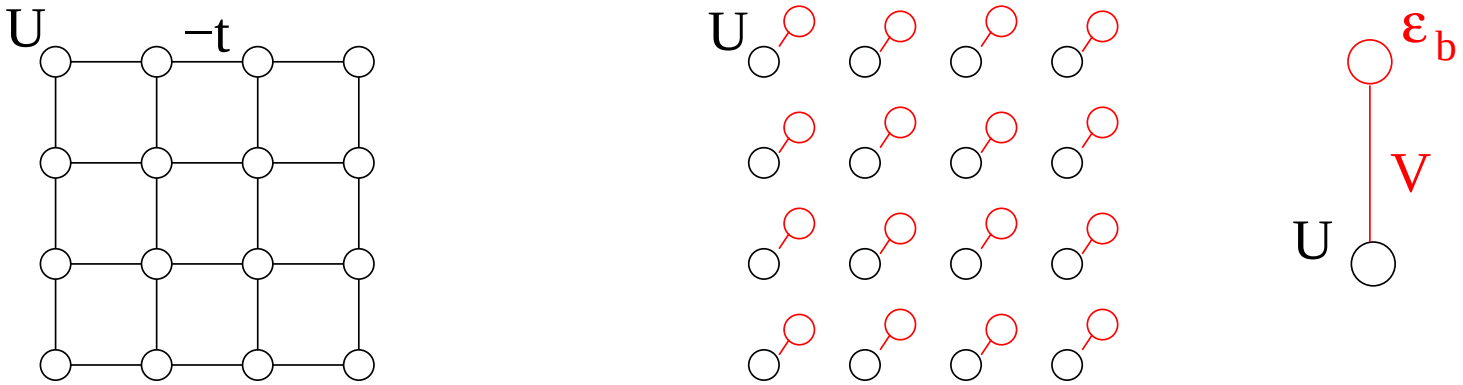
Under the transformation $c^\dagger \leftrightarrow c$ we have $n_i - 1 \longrightarrow 1 - n_i \longrightarrow$ the interaction term does not change

The kinetic term changes sign: $t_{ij} \longrightarrow -t_{ij}$ (assuming $t_{ii} = 0$)

If the lattice is bipartite and the hopping $t_{ij}$ connects only sites on different sublattices this can be compensated by a gauge transformation on one sublattice $c^\dagger_{i,\sigma} \longrightarrow -c^\dagger_{i,\sigma}$

At half-filling (1 electron/site) this transformation exchanges photoemission and inverse photoemission spectrum and implies $\mu = U/2$.

As reference system we decorate each lattice site by a noninteracting 'bath orbital' and obtain an array of dimers




The Hamiltonian for one dimer is (with $n_c = c_\uparrow^\dagger c_\uparrow + c_\downarrow^\dagger c_\downarrow$)

$$\tilde{H} - \mu N \;=\; -V \sum_\sigma (c_\sigma^\dagger b_\sigma + b_\sigma^\dagger c_\sigma) + (\epsilon_b - \frac{U}{2}) \sum_\sigma b_\sigma^\dagger b_\sigma + \frac{U}{2}\,(n_c - 1)(n_c - 1) - \frac{U}{2}$$

The transformation $c^\dagger \leftrightarrow c$, $b^\dagger \leftrightarrow -b$ transforms $\tilde{H} - \mu N$ into itself *except* for the second term.

If we put $\epsilon_b = \frac{U}{2} \rightarrow$ this term vanishes - the only remaining parameter to be varied is $V$:

$$\tilde{H} - \mu N \;=\; -V \sum_\sigma (c_\sigma^\dagger b_\sigma + b_\sigma^\dagger c_\sigma) + \frac{U}{2}\,(n_c - 1)(n_c - 1) - \frac{U}{2}$$

$$\tilde{H} - \mu N \;=\; -V \sum_{\sigma} (c_\sigma^\dagger b_\sigma + b_\sigma^\dagger c_\sigma) + \frac{U}{2}\,(n_c - 1)(n_c - 1) - \frac{U}{2}$$

All eigenstates for $0 \longrightarrow 4$ electrons can be obtained easily and $\tilde{\Omega}$ be calculated

We assume that the lattice Hamiltonian has a semi-elliptical density of states

(Width $4$, which defines the energy scale)

$$\rho_0(\epsilon) \;=\; \frac{1}{2\pi}\sqrt{4 - \epsilon^2}$$

At $T = 0$ the self-energy of the 'Hubbard orbital' can be evaluated analytically

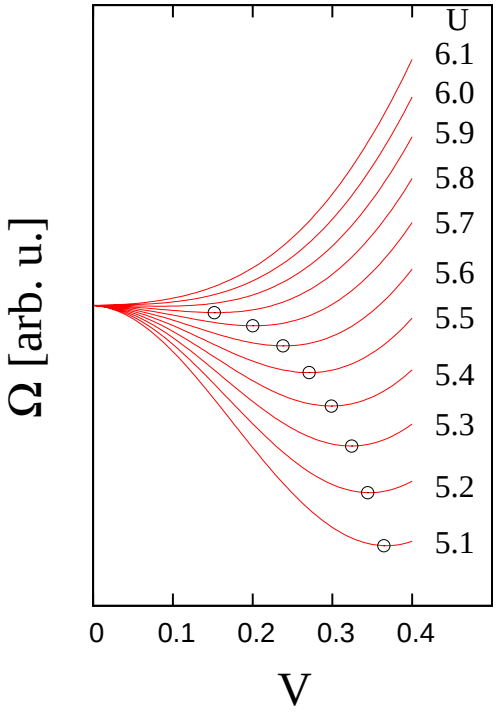
$$\Sigma(\omega) \;=\; \frac{U}{2} + \frac{U^2}{8}\left(\frac{1}{\omega + 3V} + \frac{1}{\omega - 3V}\right)$$

The $\boldsymbol{k}$-integrated Green's function of the lattice then is (remember: $\mu = \frac{U}{2}$)

$$\sum_{\mathbf{k}} G(\mathbf{k}, \omega) \;=\; \int_{-2}^{2} d\epsilon\, \frac{\rho_0(\epsilon)}{\omega + \frac{U}{2} - \epsilon - \Sigma(\omega)}$$

$$\sum_{\mathbf{k}} \ln\left(-G^{-1}(\mathbf{k}, \omega)\right) \;=\; \int_{-2}^{2} d\epsilon\, \rho_0(\epsilon)\, \ln\left(-\omega - \frac{U}{2} + \epsilon + \Sigma(\omega)\right)$$

The resulting $\Omega_{latt}(V)$ curve at $T = 0$ then looks like this




Reminder: the equation we need to solve is

$$\frac{\partial \Omega_{latt}}{\partial V} = 0$$

For $U \approx 5.85$ (remember: the width of the noninteracting band was $W = 4$) there is a phase transition finite $V \rightarrow V = 0$ - this is the metal insulator transition

Noninteracting density of states

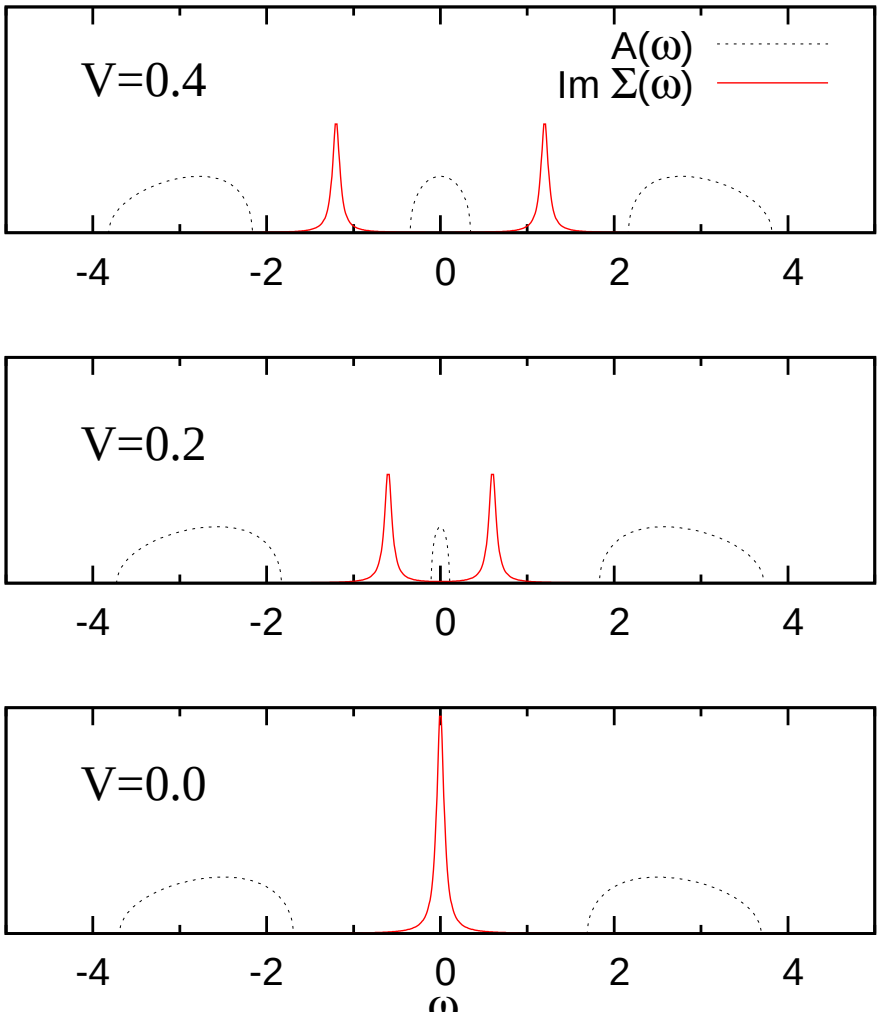
$$\rho_0(\epsilon) \;=\; \frac{1}{2\pi}\sqrt{4-\epsilon^2}.$$

Self-energy of the dimer

$$\Sigma(\omega) \;=\; \frac{U}{2} + \frac{U^2}{8}\left(\frac{1}{\omega+3V} + \frac{1}{\omega-3V}\right).$$

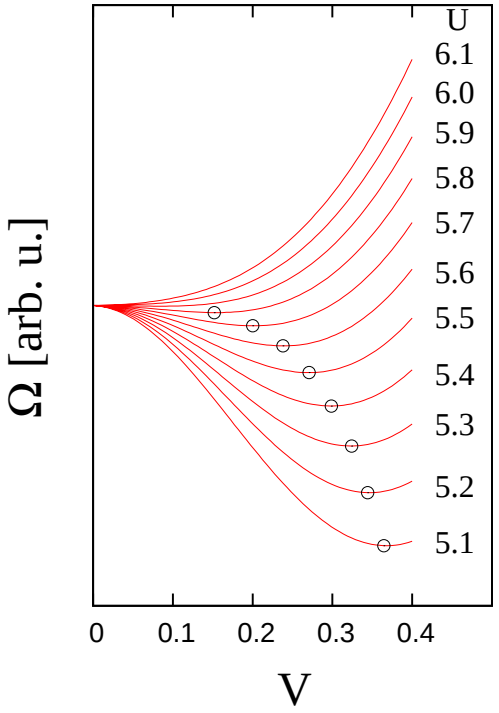
The spectral function is

$$\begin{aligned} A(\omega) \;&=\; -\Im\, G(\omega + i0^+) \\ &=\; \int_{-2}^{2} d\epsilon\, \frac{\rho_0(\epsilon)}{\omega + \frac{U}{2} - \epsilon - \Sigma(\omega+i0^+) + i0^+} \end{aligned}$$




The density of states at the Fermi surface drops to zero exactly when the two peaks merge, i.e. $V = 0$

The resulting $\Omega_{latt}(V)$ curve at $T = 0$ then looks like this

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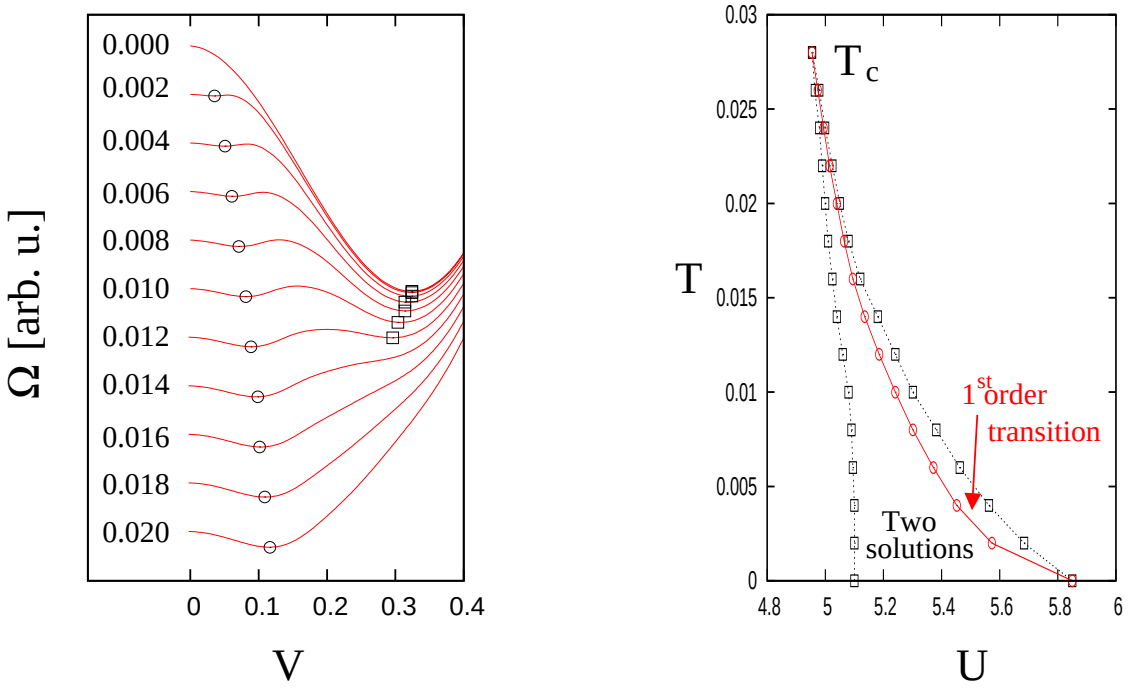
This is exactly the scenario for the metal-insulator transition familiar from DMFT calculations - but here obtained from a dimer

The critical value $U_c$ where the transition occurs is suprisingly accurate:

Dimer-VCA: $U_c = 5.85$

DMFT : $U_c = 5.84$ (G. Moeller *et al.* Phys. Rev. Lett. $\mathbf{74}$, 2082 (1995))

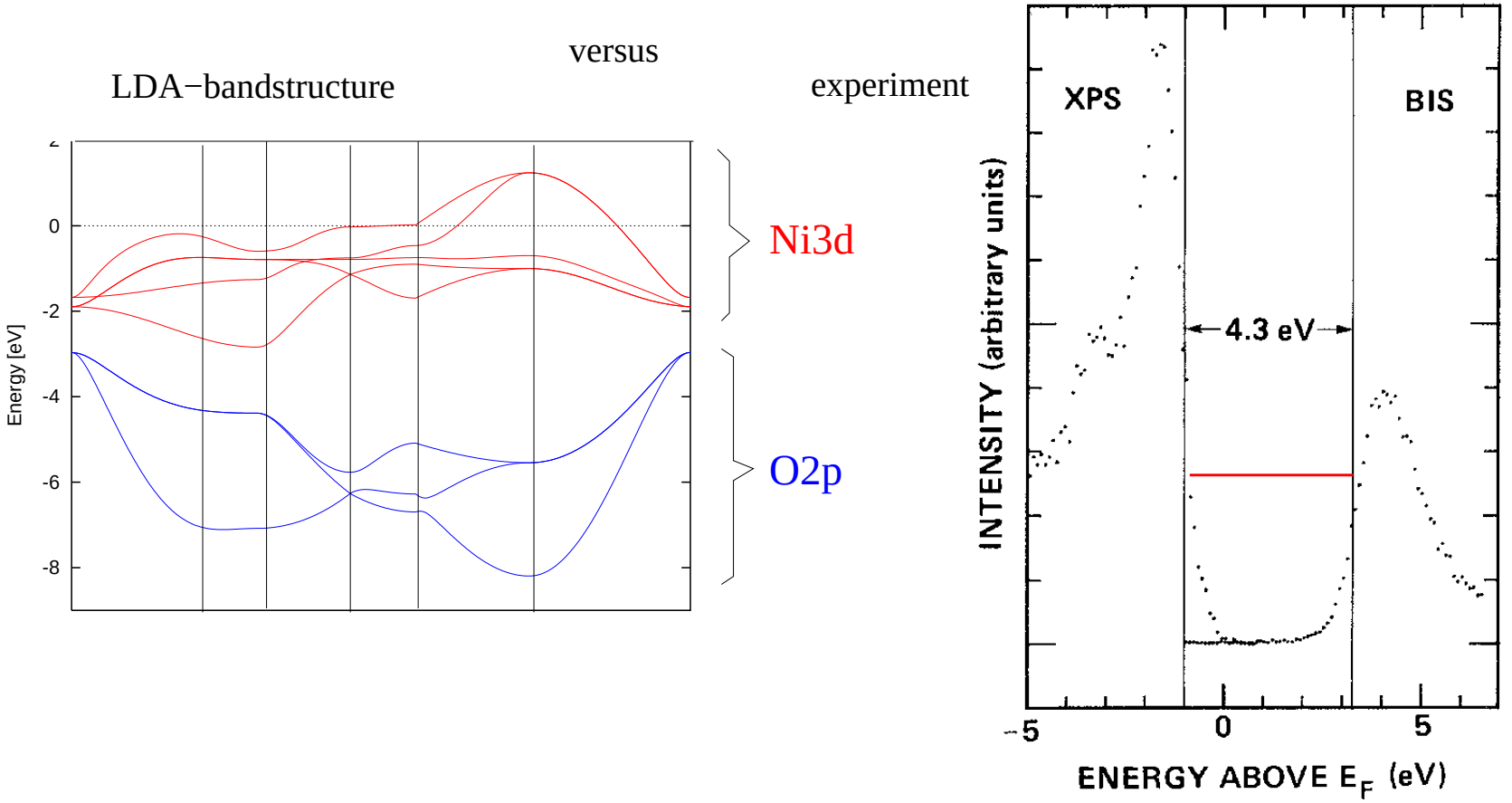
At finite temperature the VCA shows a more complicated behaviour




Finite region of coexistence of metallic and insulating solution with $1^{st}$ order transition between the two

# Electronic structure calculations for transition metal compounds

LDA band structure calculations often do not reproduce the single-particle spectra of correlated insulators

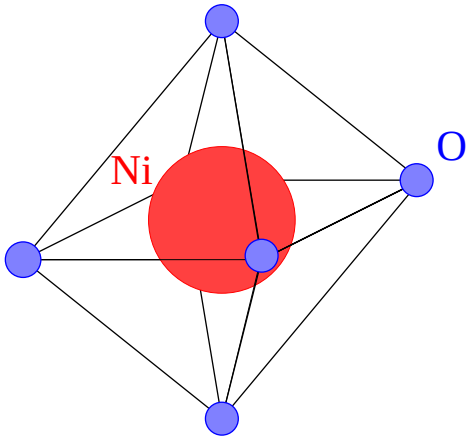


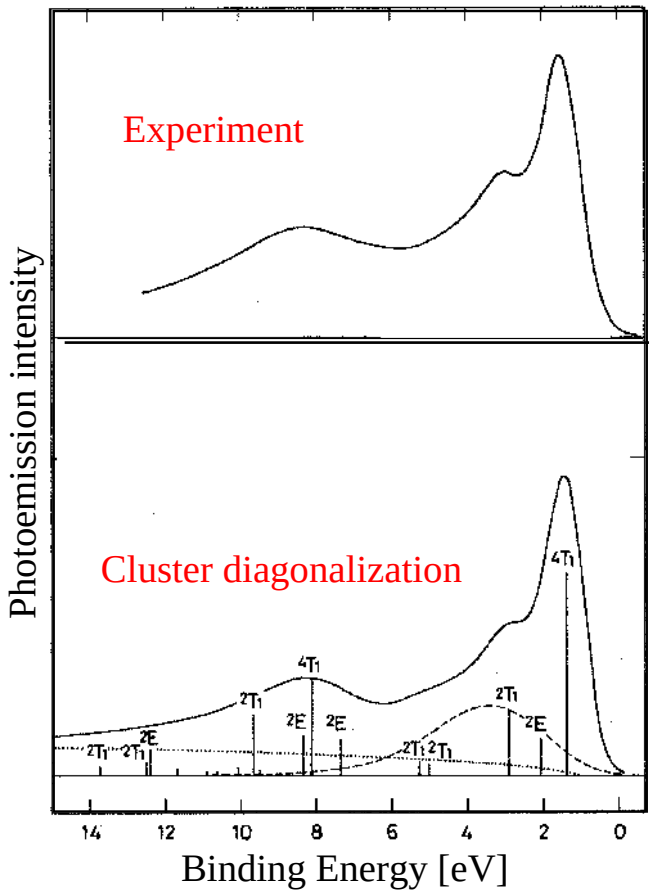

Experiment: G. A. Sawatzky and J. W. Allen, Phys. Rev. Lett. **53**, 2239 (1984).

# The cluster method

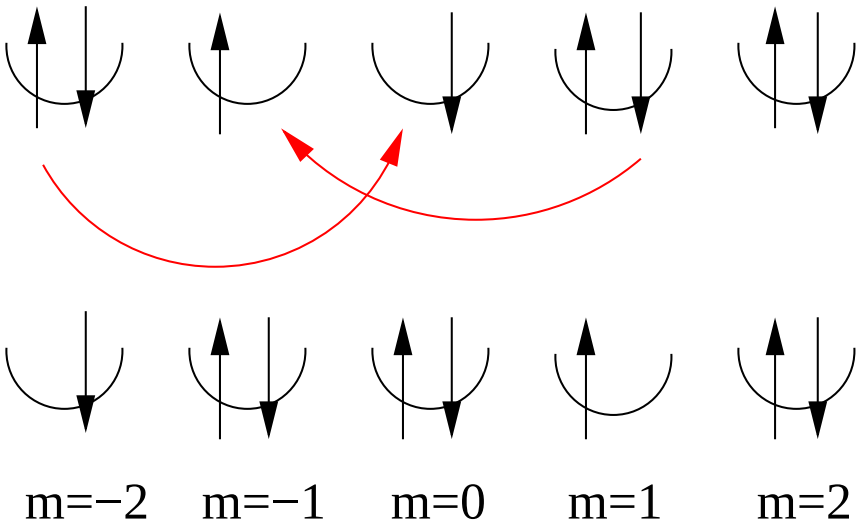
Angle integrated photoemission spectra of TM oxides can be described very well by exact diagonalization of a single TM-Ion in a 'cage' of oxygen ligands (cluster)

Example: Valence band photoemission spectrum of NiO (Fujimori and Minami, Phys. Rev. B **30**, 957 (1984))



Crucial ingredient: the full Coulomb interaction in the 3d-shell




- Electrons in a partially filled shell scatter from each other due to their Coulomb interaction
- This amounts to a redistribution of the electrons within the partially filled shell
- For $L^z$ to be conserved the scattering electrons must 'move along the m-ladder' in exactly opposite ways

Calculation of the Coulomb matrix element

$$V = \int d\mathbf{r}\, d\mathbf{r}'\; \Psi_1^*(\mathbf{r})\Psi_2^*(\mathbf{r}')\; \frac{1}{|\mathbf{r}-\mathbf{r}'|}\; \Psi_3(\mathbf{r})\Psi_4(\mathbf{r}')$$

Now insert ($l_1 = l_2 = l_3 = l_4 = 2$)

$$\Psi_1^*(\mathbf{r})\Psi_2^*(\mathbf{r}') \;=\; R_d(r)\; Y^*_{l1,m1}(\Theta,\phi)\;\; R_d(r')\; Y^*_{l2,m2}(\Theta',\phi')$$

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} \;=\; \sum_{l,m} Y^*_{l,m}(\Theta,\phi)\;\; \frac{r_<^l}{r_>^{l+1}} \;\; Y_{l,m}(\Theta',\phi')$$

$$\Psi_3(\mathbf{r})\Psi_4(\mathbf{r}') \;=\; R_d(r)\; Y_{l3,m3}(\Theta,\phi)\;\; R_d(r')\; Y_{l4,m4}(\Theta',\phi')$$

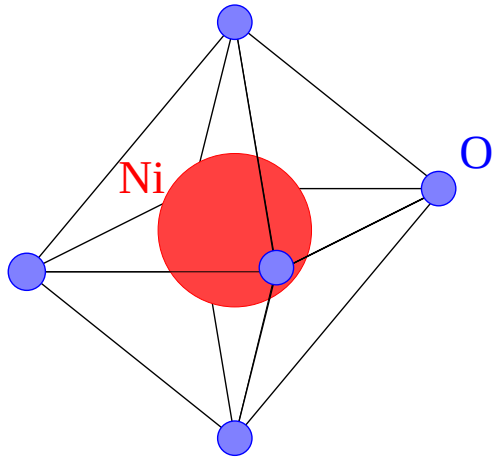
and obtain

$$V \;=\; \sum_{l,m} \int d\Omega\; Y^*_{l1,m1}(\Theta,\phi)\; Y^*_{l,m}(\Theta,\phi)\; Y_{l3,m3}(\Theta,\phi) \qquad \int d\Omega'\; Y^*_{l2,m2}(\Theta',\phi')\; Y_{l,m}(\Theta',\phi')\; Y_{l4,m4}(\Theta',\phi')$$

$$\int_0^\infty dr \int_0^\infty dr'\; R_d(r)R_d(r')\; \frac{r_<^l}{r_>^{l+1}}\; R_d(r)R_d(r')$$

- Expressible in terms of Gaunt coefficients (tabulated) and Slater integrals $I_l$ (easily computed)

The cluster:




The Hamiltonian:

$$H = \frac{1}{2}\sum_{i,j,k,l} V(\nu_i,\nu_j,\nu_k,\nu_l)\; c^\dagger_{\nu_i}\, c^\dagger_{\nu_j}\, c_{\nu_k}\, c_{\nu_l} + \sum_{i,j} V_{CEF}(\nu_i,\nu_j)\; c^\dagger_{\nu_i} c_{\nu_j}$$
$$+ \sum_{i,j}\left(t_{\nu_i,\mu_j}\; c^\dagger_{\nu_i}\; l_{\mu_j} + H.c.\right) + \sum_j\; \epsilon_{\mu_j}\; l^\dagger_{\mu_j} l_{\mu_j} + \sum_i\; \epsilon_{\nu_i}\; c^\dagger_{\nu_i} c_{\nu_i}$$

This comprises the Coulomb interaction in the TM 3d-shell, the Crystalline electric field, the charge transfer between TM 3d-shell and ligands, and the orbital energies of transition metal d-orbitals and ligands

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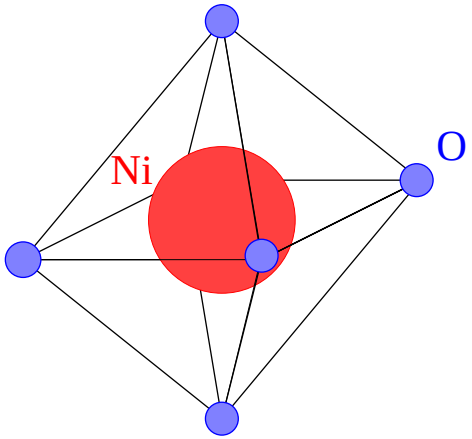
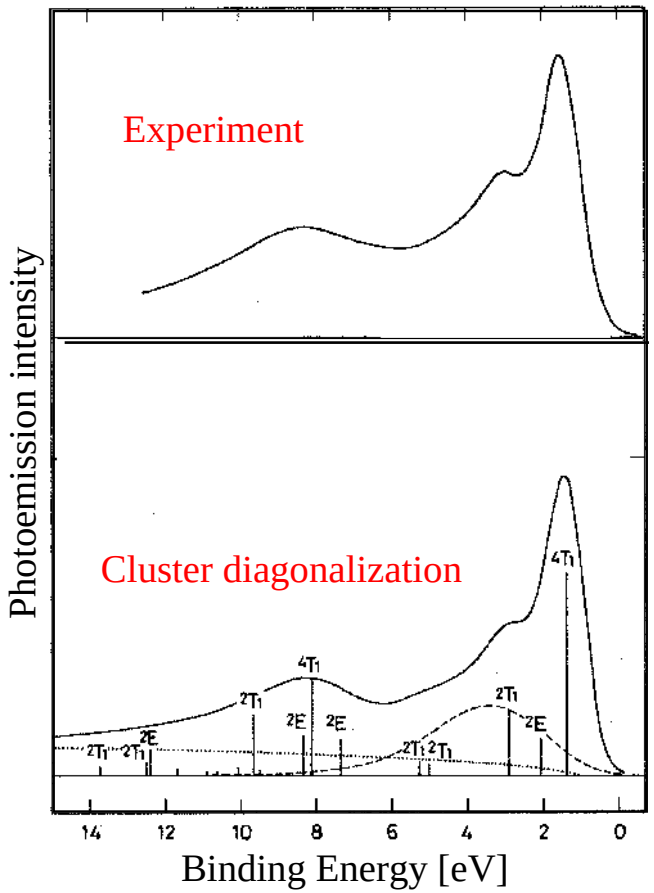
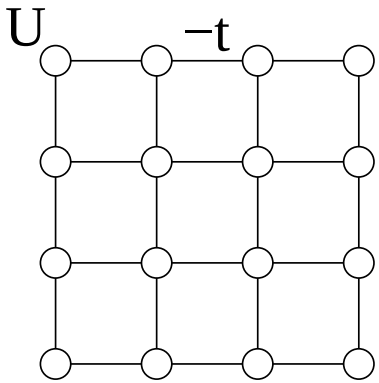
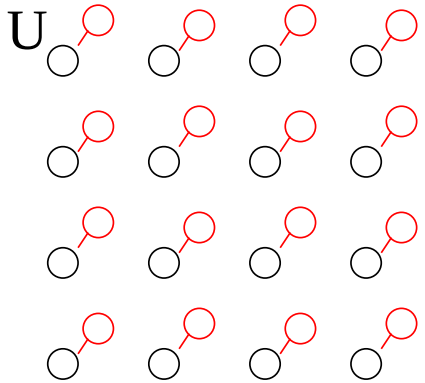


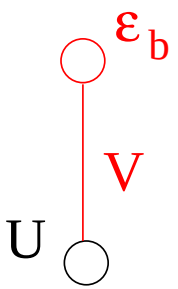



## VCA treatment of transition metal compounds

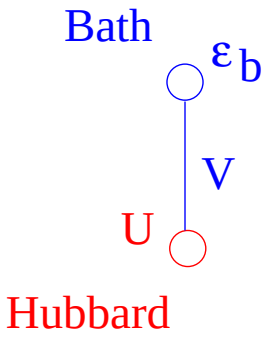
Reminder: In the dimer-VCA of the Hubbard model we used simple dimers to generate self-energies

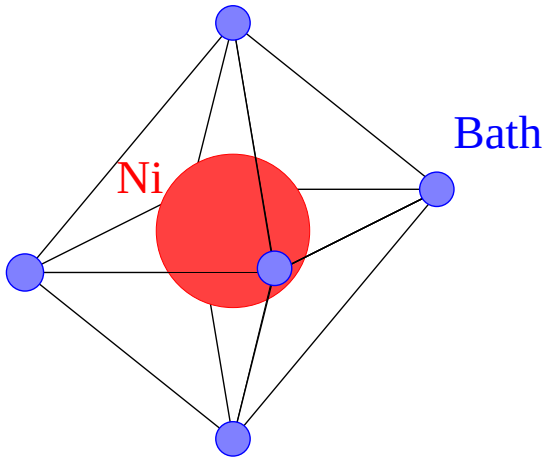


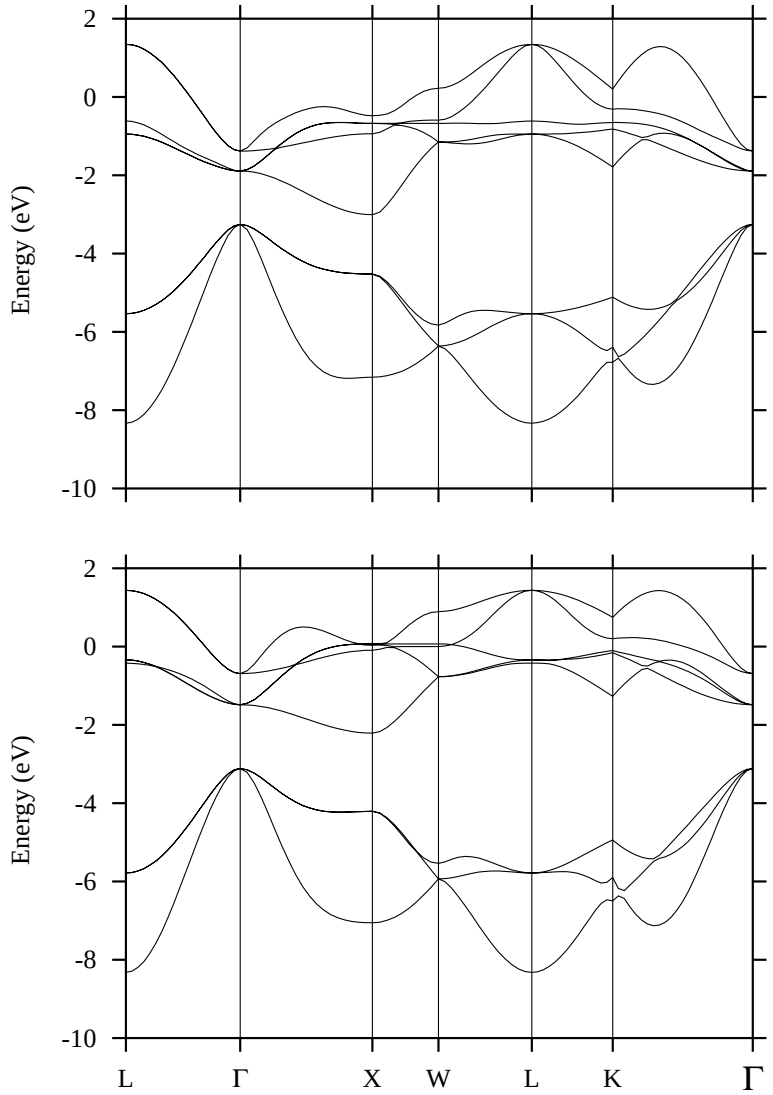

The most obvious generalization is to use octahedral clusters with $10$ orbitals instead of the dimers



## Some technical points

The noninteracting $\mathbf{t}(\mathbf{k})$ is obtained by an LCAO-fit (bottom) to an LDA band structure (top)



## Some technical points

The Slater integral $I_0$ is strongly screened in the solid

The orbital energy $e_d$ obtained by fit to the LDA-bandstructure 'contains' the $d-d$ Coulomb interaction (Hartree potential plus $V_{xc}$)

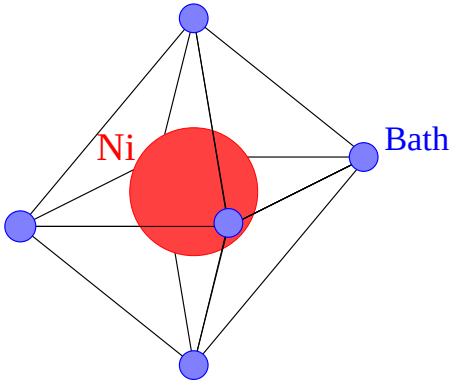
On the other hand the Hartree-Fock-potential is contained in the self-energy of the cluster:

$$\Sigma(\omega) = V_{HF} + \sum_{\nu} \frac{A_\nu}{\omega - B_\nu}$$

To avoid double counting $e_d$ must be corrected for (a mixture of) $V_{HF}$ and $V_{xc}$

For simplicity $I_0$ and the 'bare' d-level energy $\tilde{\epsilon}_d$ were adjusted to match the position of the satellite and the insulating gap!

## Some technical points



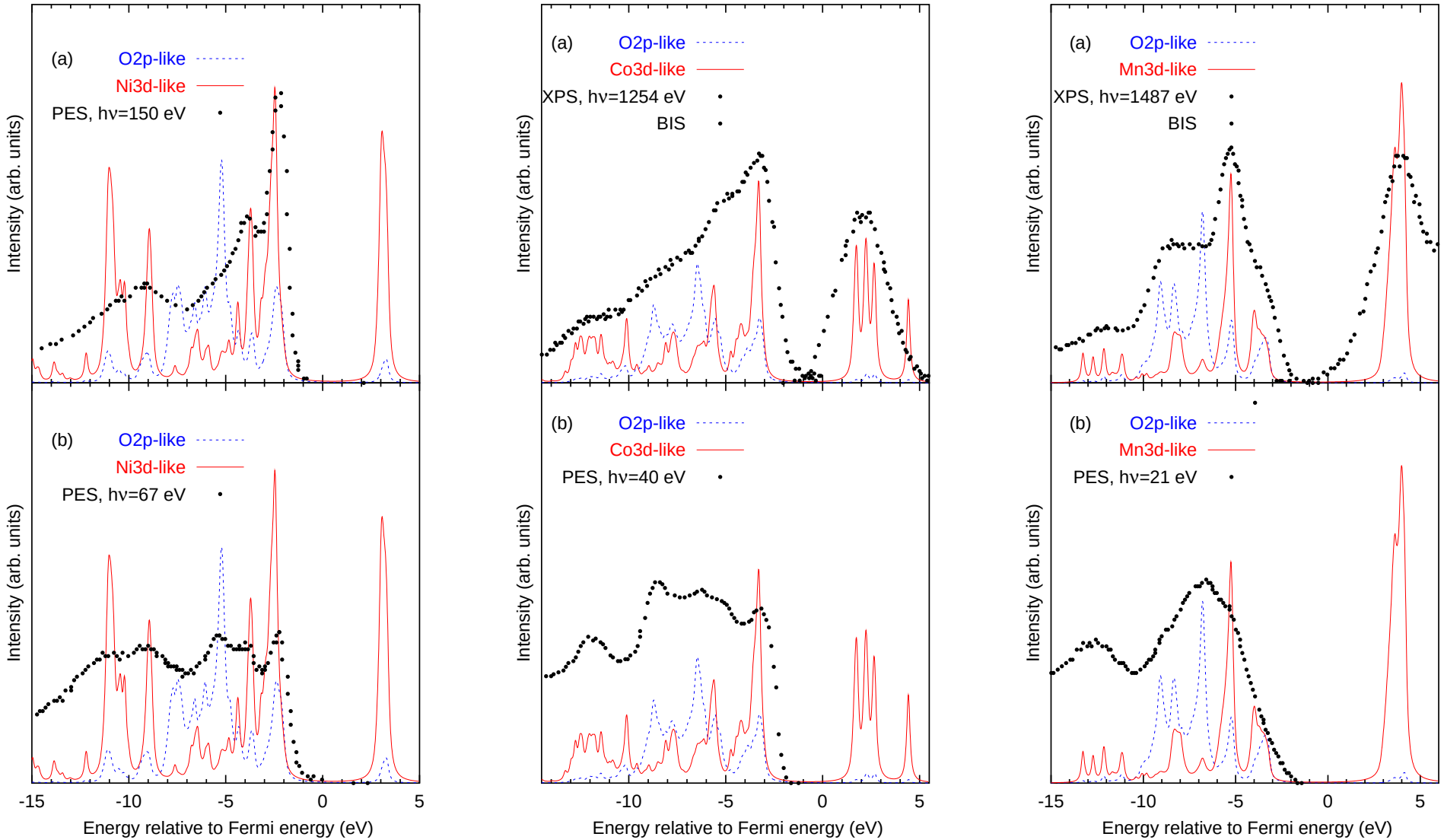

The octahedral cluster allows for a total of $6$ parameters

- 2 energies of $d$-levels ($e_g$ and $t_{2g}$)
- 2 energies of bonding Ligand combinations ($e_g$ and $t_{2g}$)
- 2 d-Level - Ligand combination hybridization integrals ($e_g$ and $t_{2g}$)

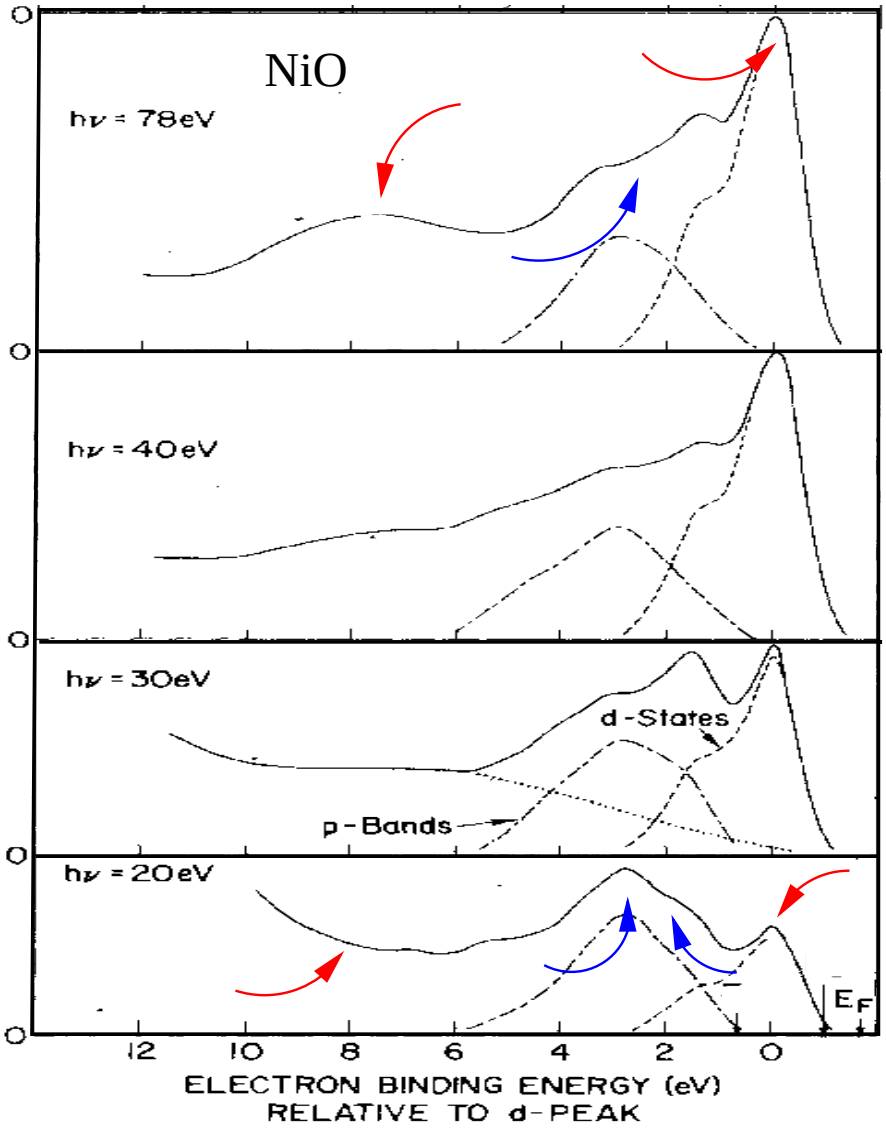
It turned out that there is a kind of 'saturation'

Optimization of more than $4$ parameters leads to extremely small change of $\delta\Omega \propto 10^{-4}\ eV$ and 'almost stationary' directions in parameter-space $\longrightarrow$ at most $4$ parameters were optimized

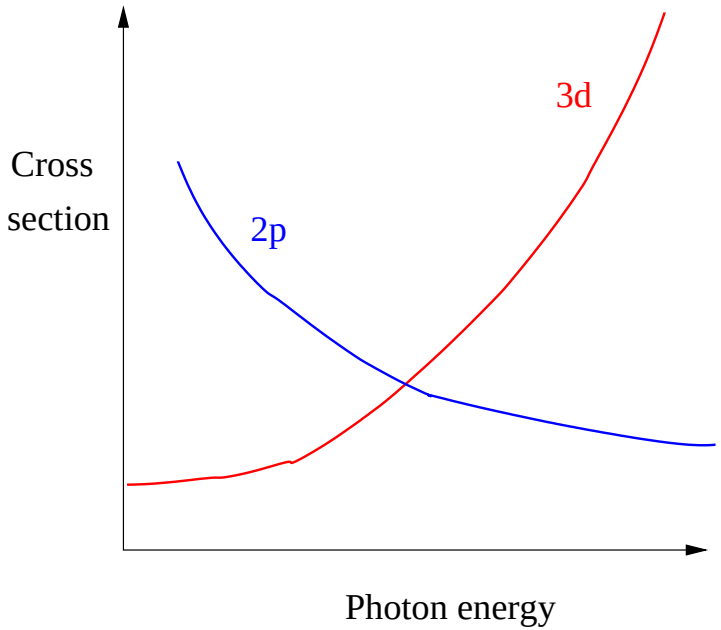
# Comparison with experiment: Angle integrated valence band photoemission spectra of NiO, CoO and MnO



# Character of states: photon energy dependence of photoelectron spectra




The mechanism of the smoother variation is the photon energy dependence of the photoionization cross section



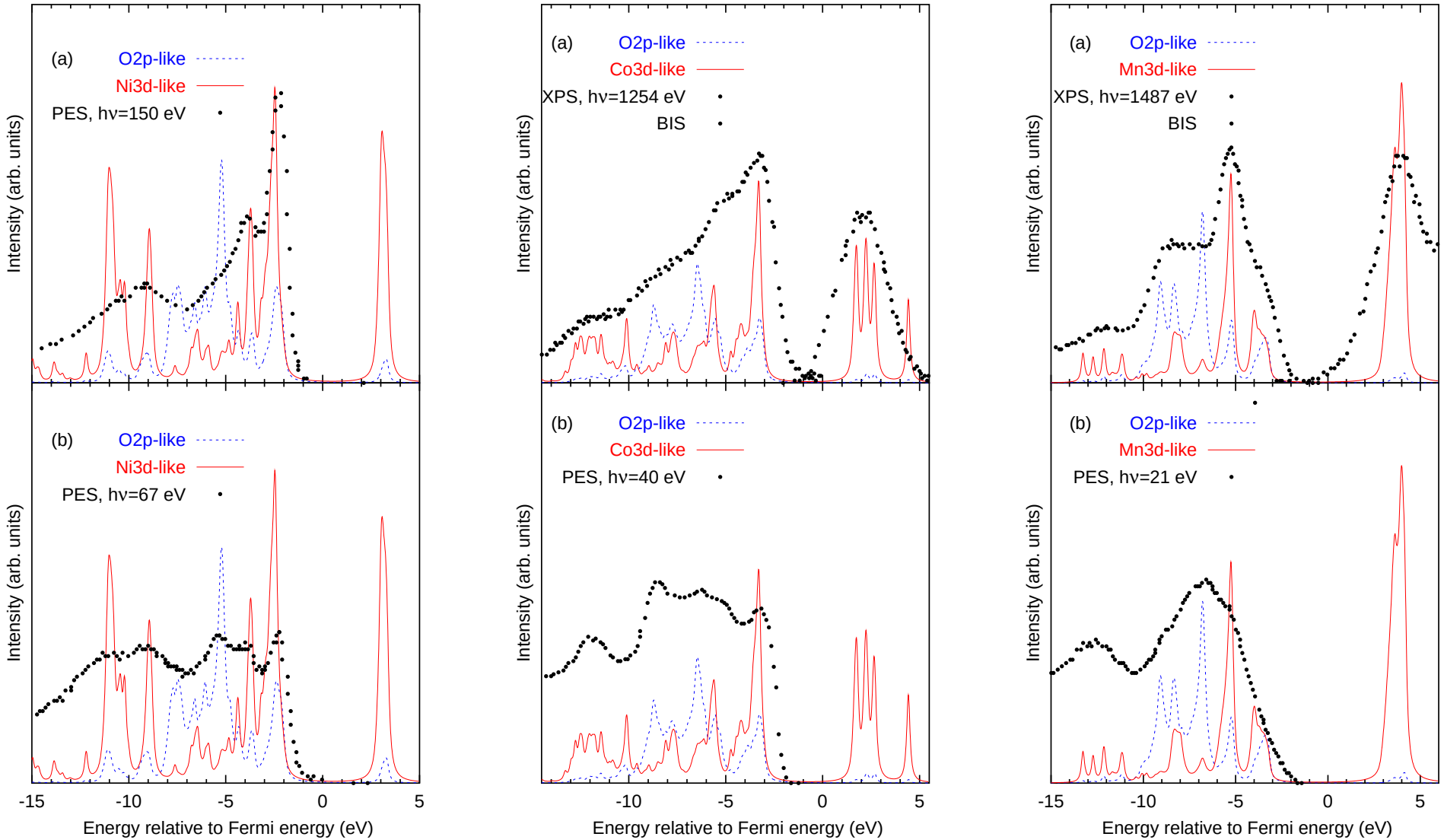

Data from Eastman & Freeouf, PRL 34, 395 (1975)

## Rule of thumb

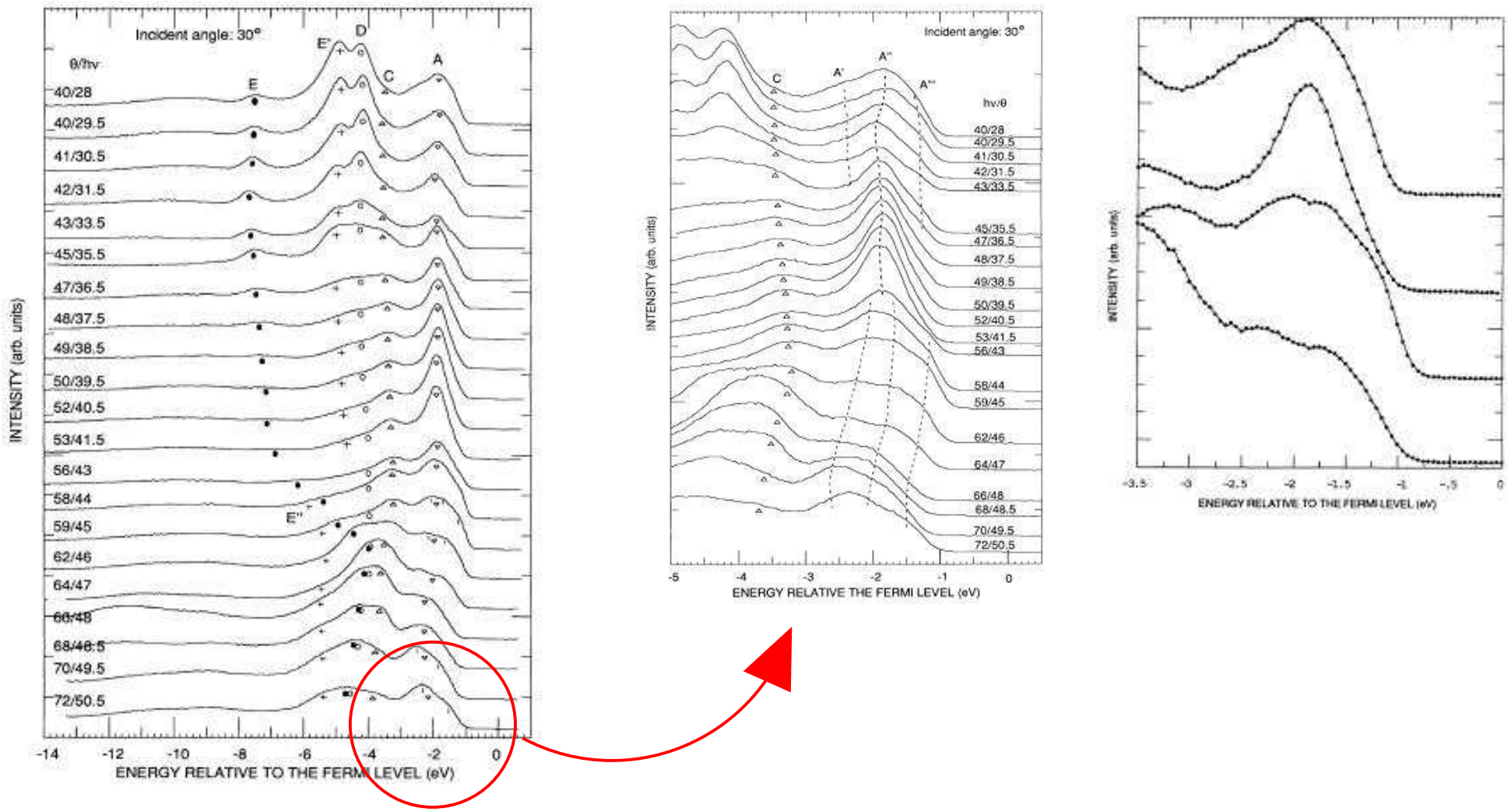
Features which increase in intensity with decreasing photon energy are O2p-derived

Features which decrease in intensity with decreasing photon energy are metal 3d-derived

# Comparison with experiment: Angle integrated valence band photoemission spectra of NiO, CoO and MnO



Experimental band structure of NiO (Z. X. Shen *et al.*, Phys. Rev. B **44**, 3604 (1991))



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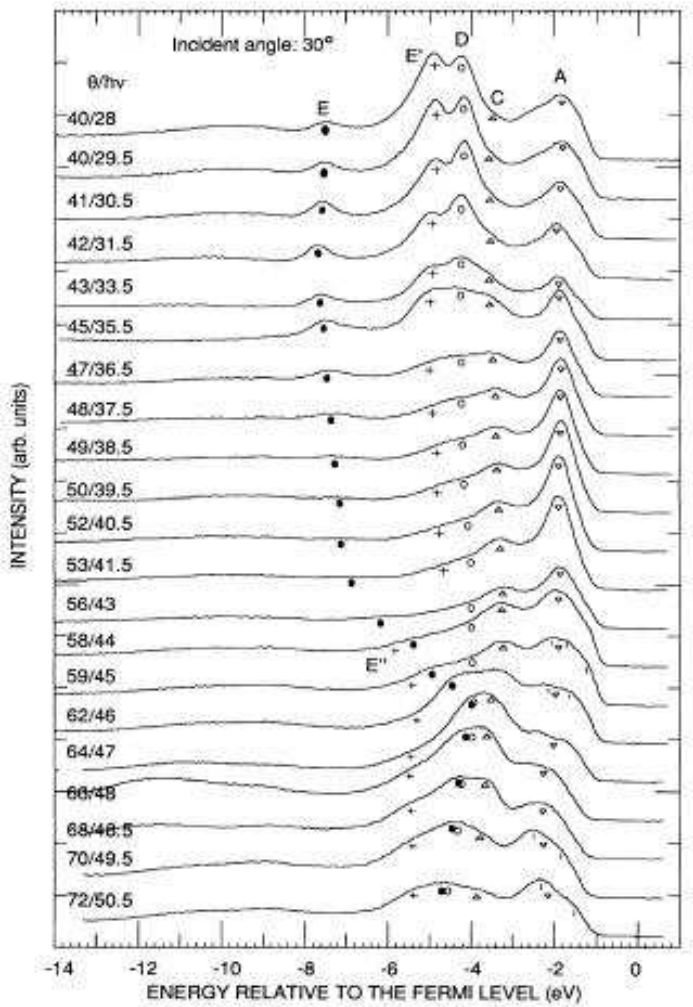
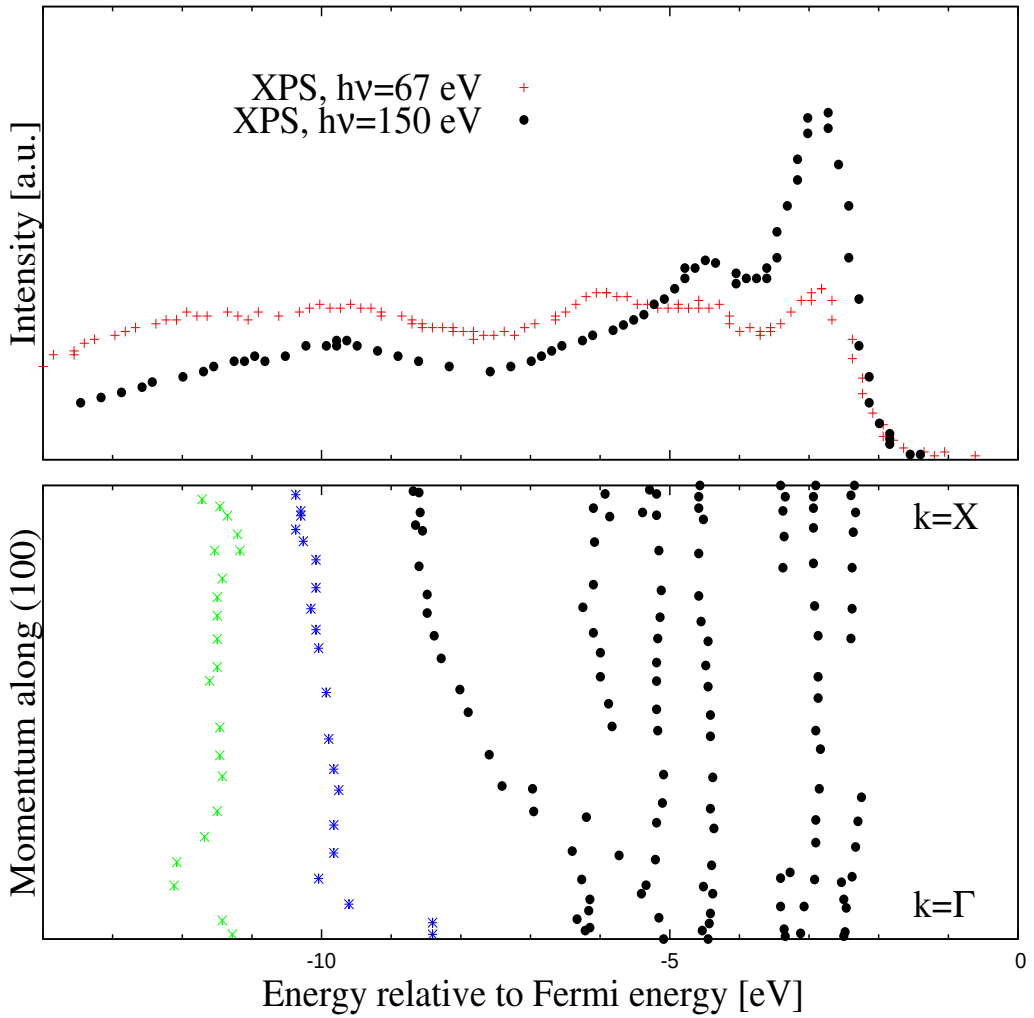
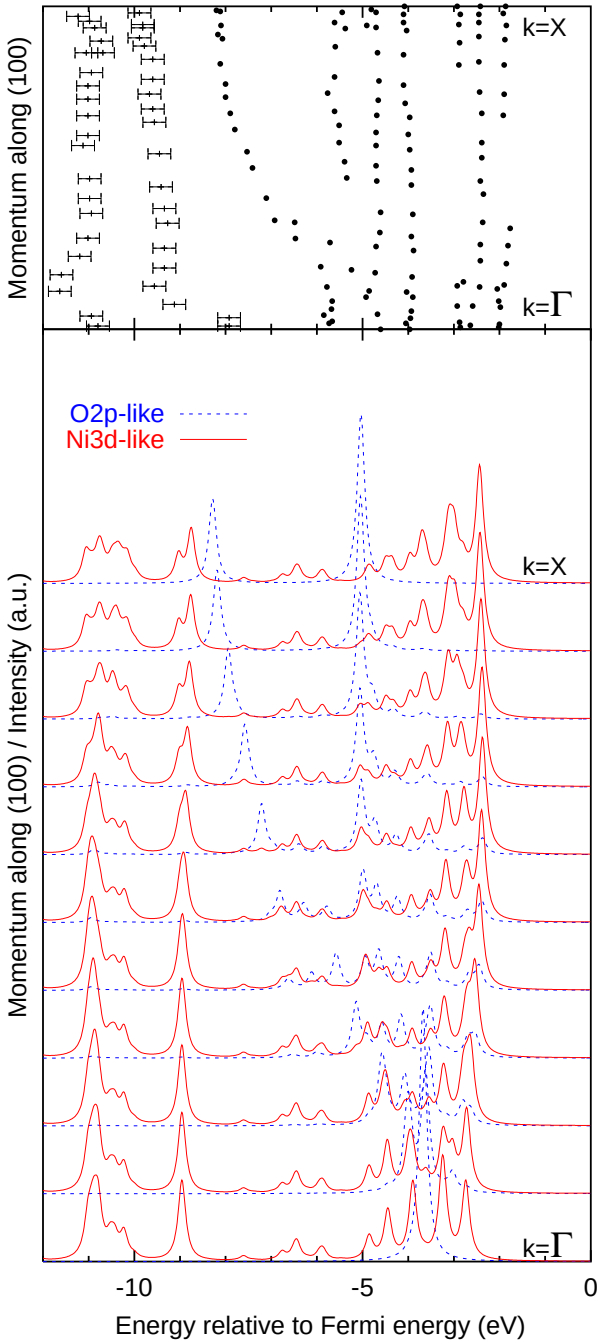
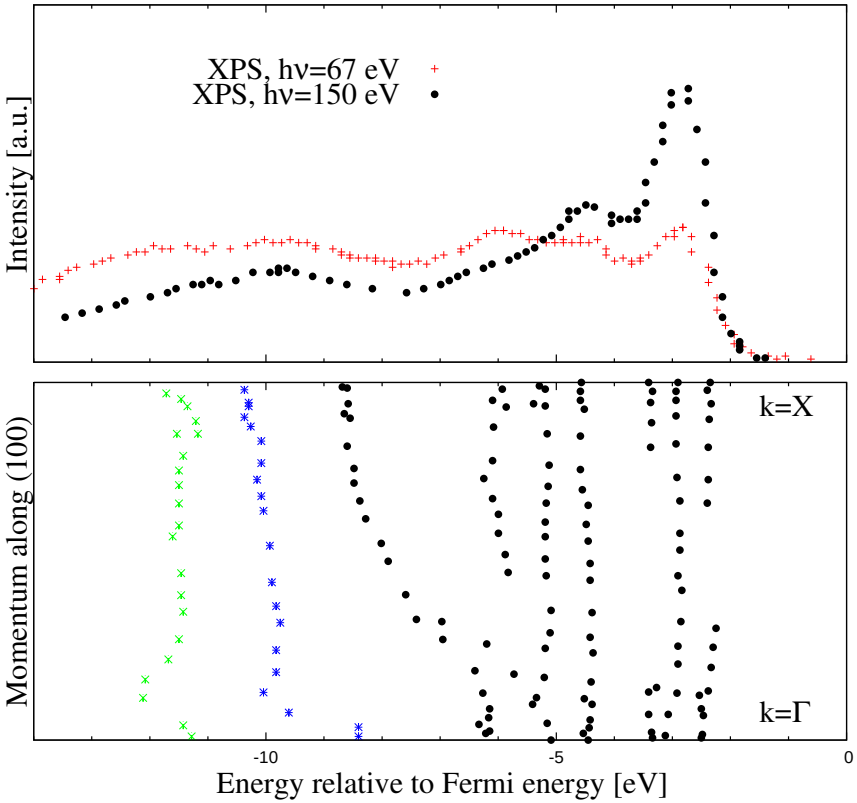
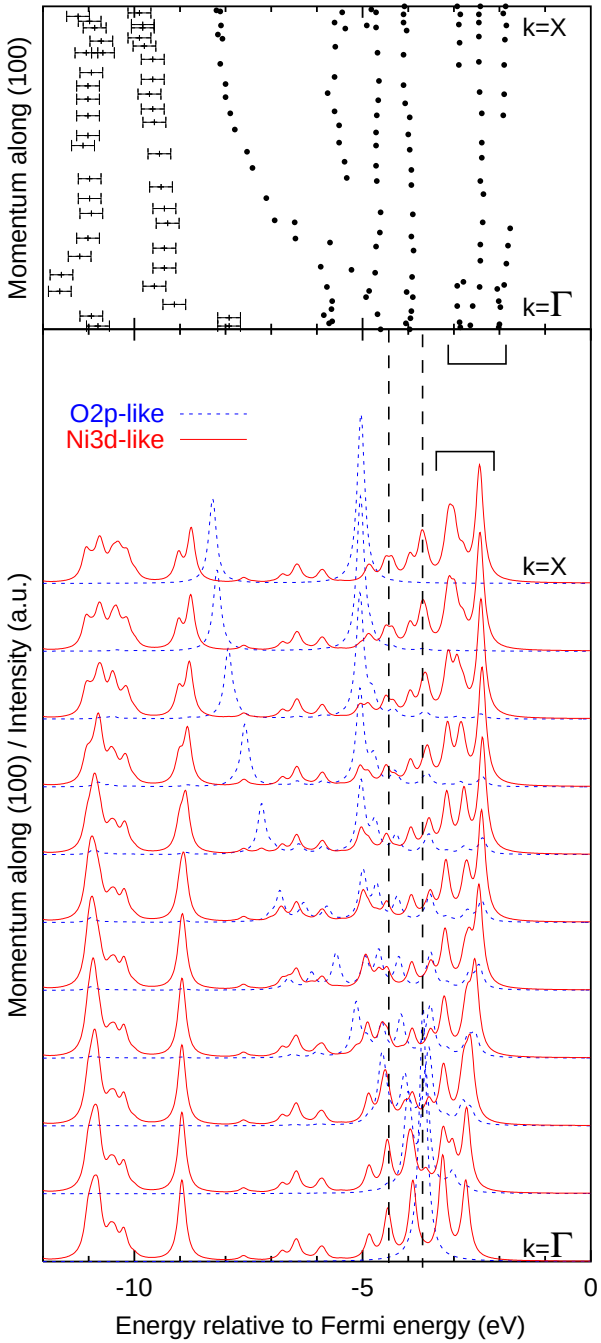
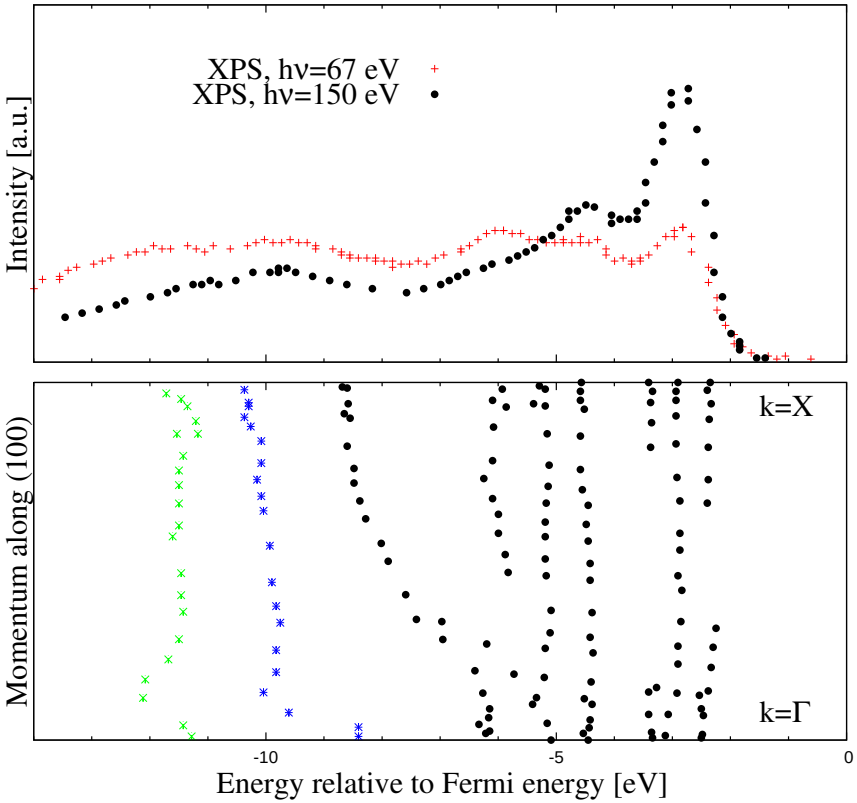


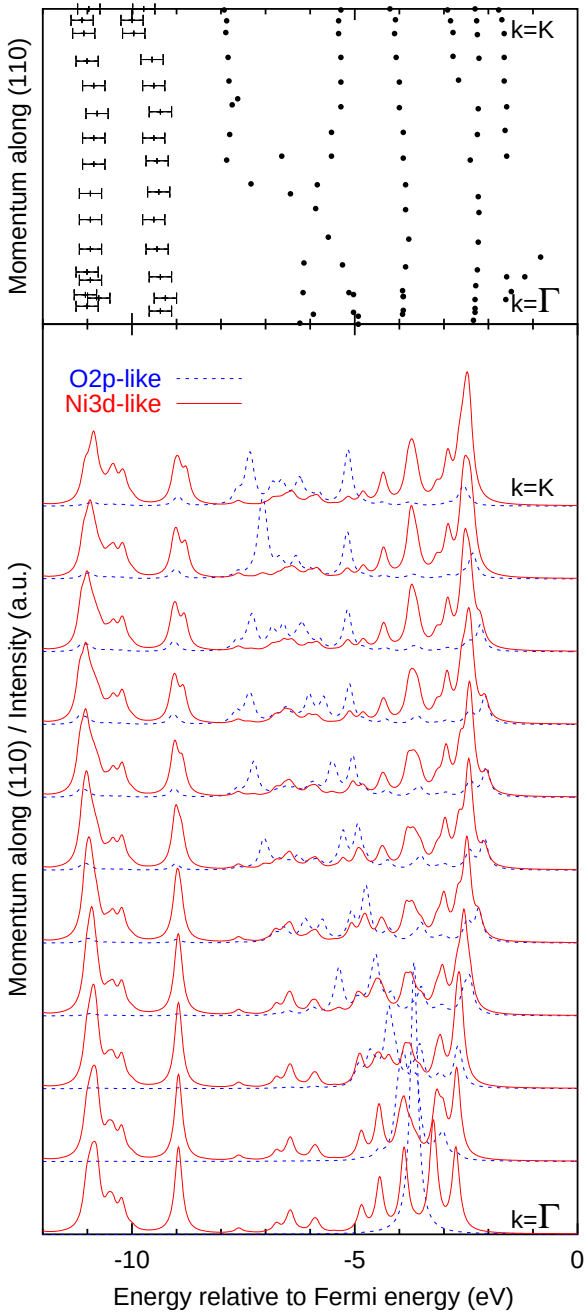




Momentum along (100)
k=X
k=Γ
O2p-like
Ni3d-like
Momentum along (100) / Intensity (a.u.)
k=X
k=Γ
-10
-5
0
Energy relative to Fermi energy (eV)

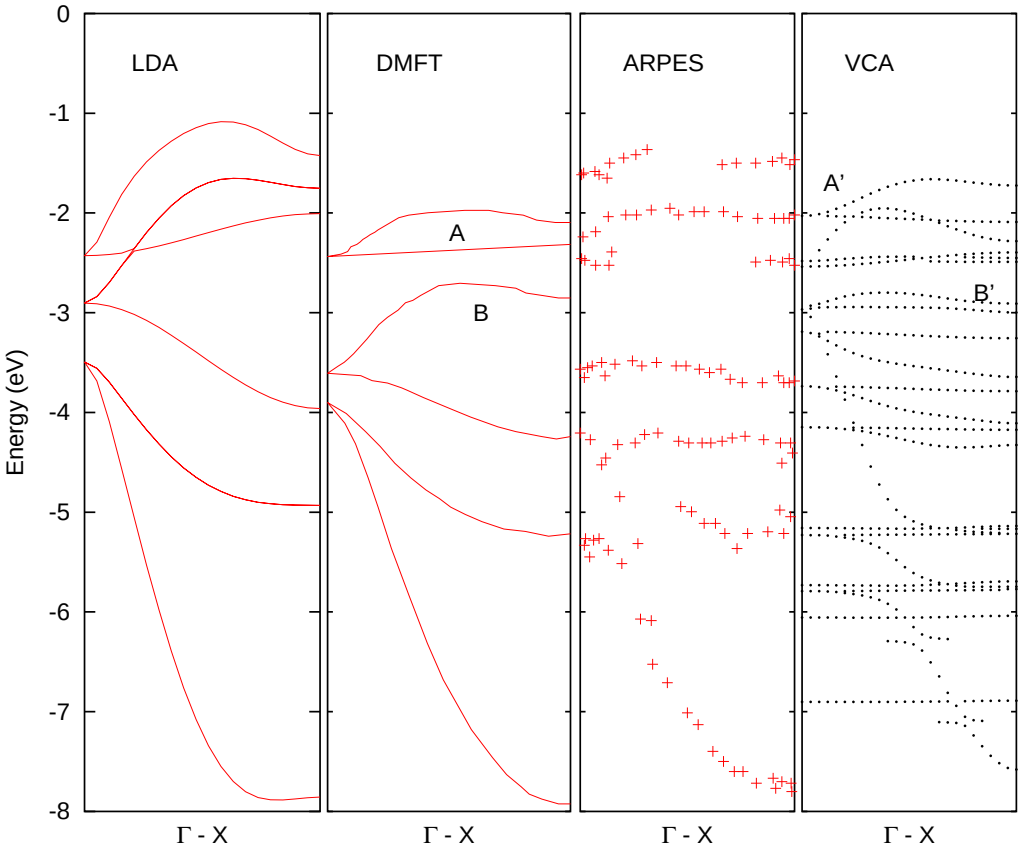

XPS, hν=67 eV
XPS, hν=150 eV
Intensity [a.u.]
Momentum along (100)
k=X
k=Γ
-10
-5
0
Energy relative to Fermi energy [eV]

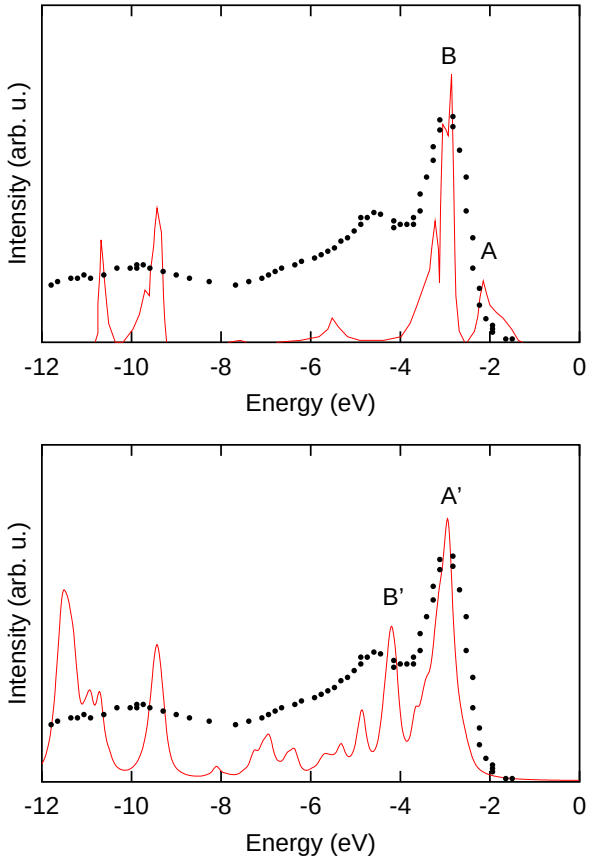

k=X
k=Γ
Momentum along (100)
O2p-like
Ni3d-like
k=X
k=Γ
Momentum along (100) / Intensity (a.u.)
-10
-5
0
Energy relative to Fermi energy (eV)


XPS, hν=67 eV
XPS, hν=150 eV
Intensity [a.u.]
k=X
k=Γ
Momentum along (100)
-10
-5
0
Energy relative to Fermi energy [eV]


Momentum along (110)
k=K
k=Γ
O2p-like
Ni3d-like
Momentum along (110) / Intensity (a.u.)
k=K
k=Γ
-10
-5
0
Energy relative to Fermi energy (eV)

Summary of bandstructure results for NiO along $(1, 0, 0)$




ARPES: Z.X. Shen *et al.*, Phys. Rev. B **44**, 3604 (1991)

DMFT: Q. Yin *et al.*, Phys. Rev. Lett. **100**, 066406 (2008)

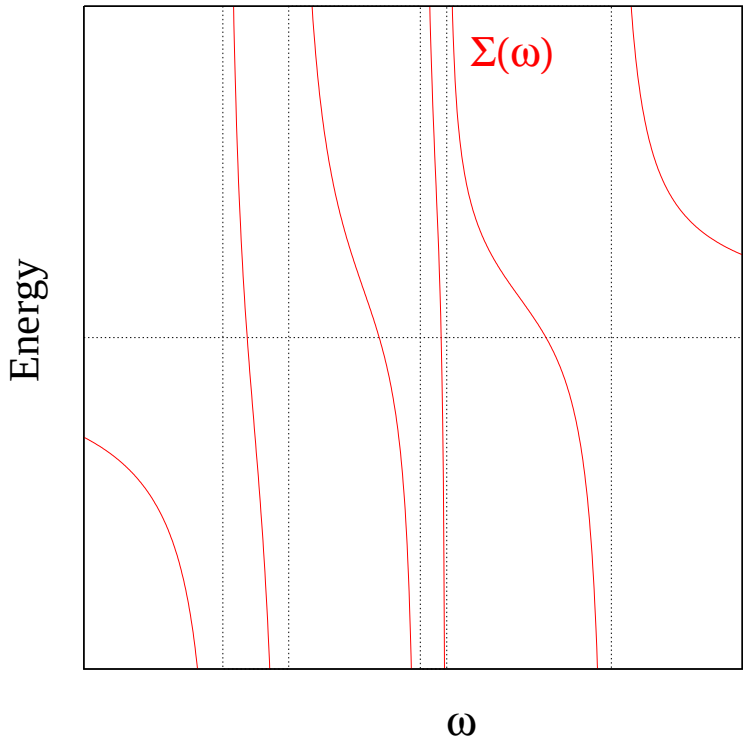
## Summary

- The Grand Canonical Potential of an interacting Fermi system can be expressed as a functional of its self-energy
- This functional is stationary at the true self-energy but contains the Luttinger-Ward functional which is impossible to evaluate for a given self-energy
- In the Variational Cluster Approximation due to Potthoff this problem is circumvented by generating self-energies by exact diagonalization of small clusters and calculate the Luttinger-Ward functional numerically
- Combining the VCA with the cluster method for transition metal oxides allows to calcuate reasonably accurate photoemisison spectra etc

## A Self-energy with more than one pole

$$\Sigma(\omega) = \eta + \sum_i \frac{\sigma_i}{\omega - \zeta_i}$$

$$\omega - \epsilon_{\mathbf{k}} = \Sigma(\omega)$$



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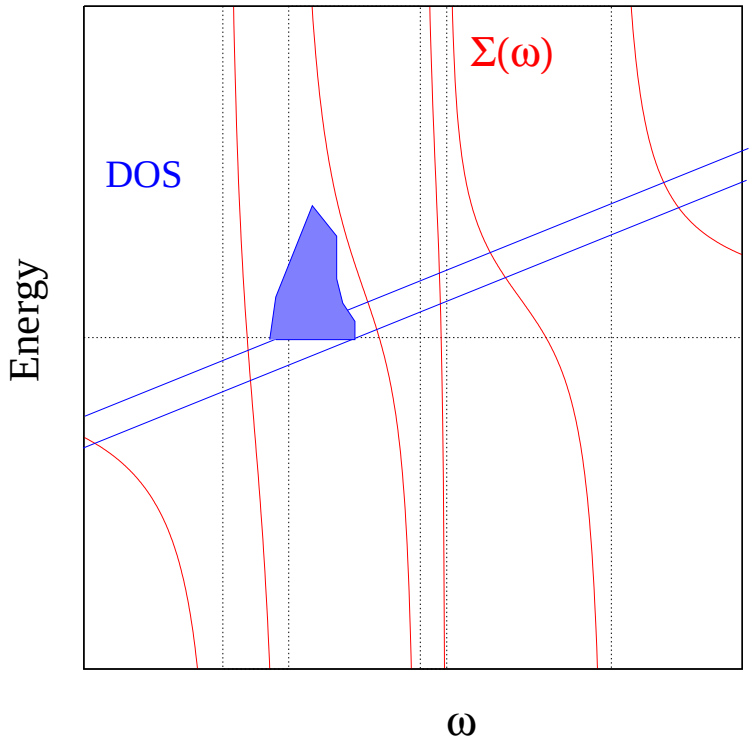

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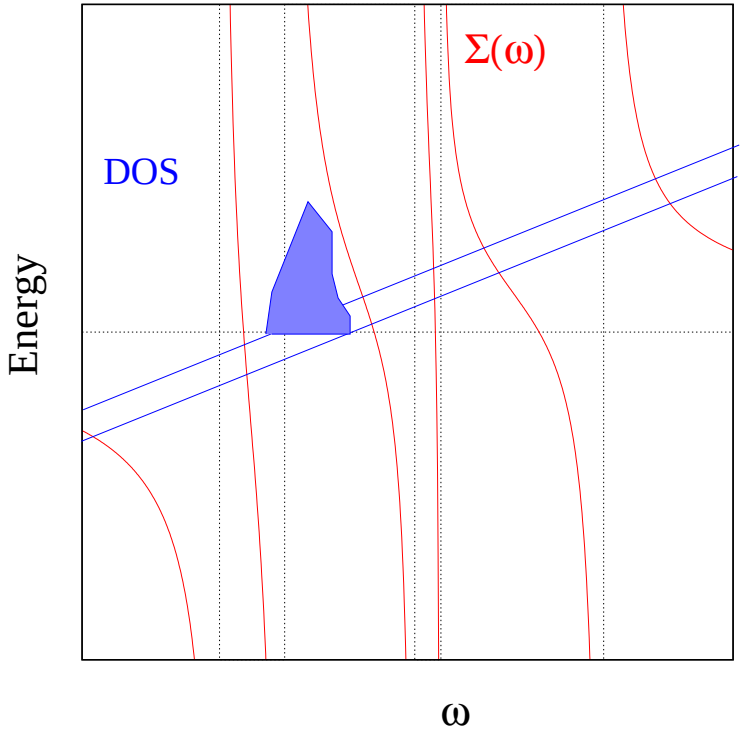


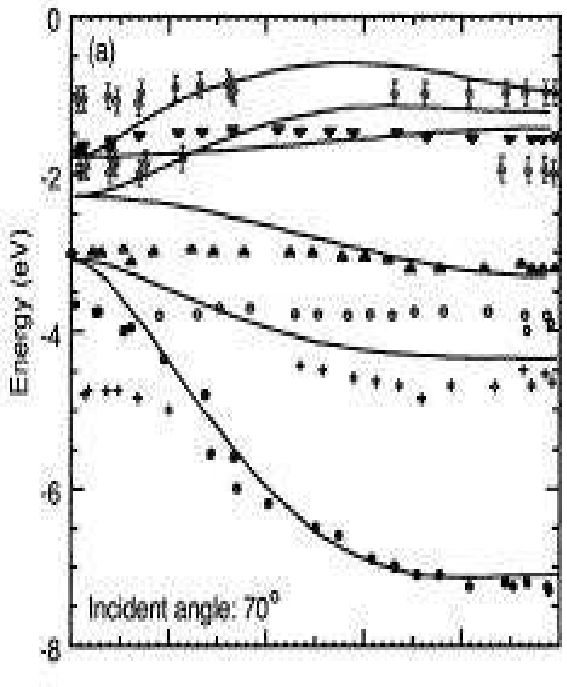

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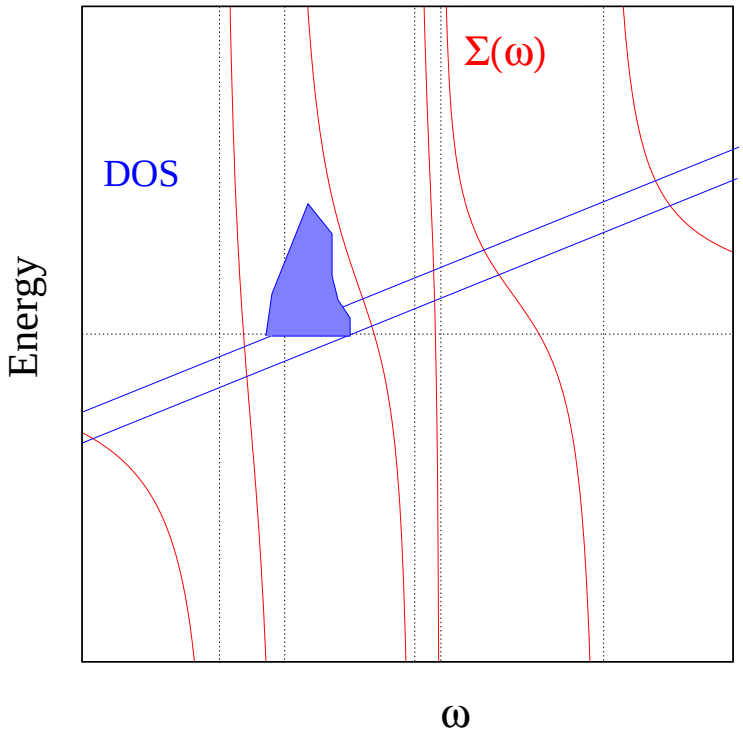


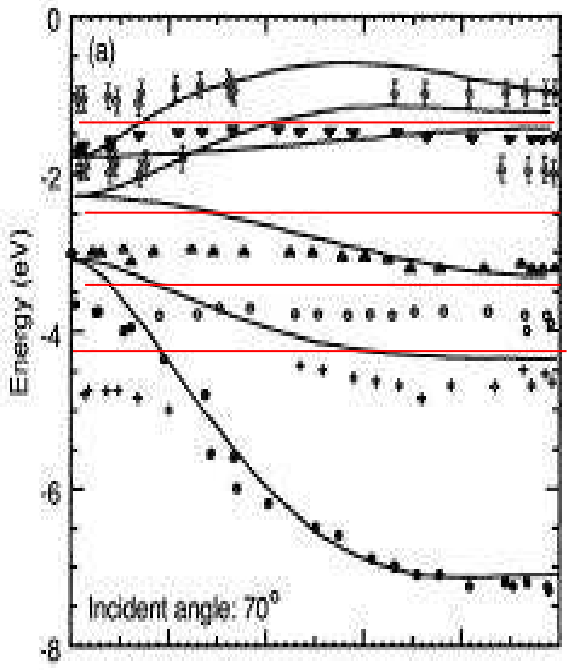

## Calculation of $\langle \lambda H_1 \rangle_\lambda$

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

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

We assume $\tau < 0$, temporarily replace $(i,\alpha) \to \alpha$ and write $H - \mu N \to K$

$$\begin{aligned} G_{\alpha,\alpha}(\tau) &= \langle c^\dagger_\alpha \;\; c_\alpha(\tau)\rangle \\ &= \langle c^\dagger_\alpha \;\; e^{\frac{\tau}{\hbar}K}\; c_\alpha\; e^{-\frac{\tau}{\hbar}K}\,\rangle \\ \to -\hbar\,\frac{\partial G_{\alpha,\alpha}(\tau)}{\partial\tau} &= \langle c^\dagger_\alpha \;\; e^{\frac{\tau}{\hbar}K}\,[c_\alpha, K]\; e^{-\frac{\tau}{\hbar}K}\,\rangle \end{aligned}$$

$$\to \lim_{\tau\to 0^-}\left(-\hbar\,\frac{\partial G_{\alpha,\alpha}(\tau)}{\partial\tau}\right) = \langle c^\dagger_\alpha \;\; [c_\alpha, K]\,\rangle$$

$$\lim_{\tau\to 0^-}\sum_i \text{trace}\left(-\hbar\,\frac{\partial G_{i,\alpha,i,\alpha}(\tau)}{\partial\tau}\right) = \sum_{i,\alpha}\langle c^\dagger_{i,\alpha} \;\; [c_{i,\alpha}, H-\mu N]\,\rangle = \langle H_0 - \mu N\rangle + 2\langle H_1\rangle$$