Quantum Cluster Methods for Strongly Correlated Electron Systems:

Variational Approach

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Advanced School of Recent Progress in
Condensed Matter Physics and Strongly Correlated Systems

IPM

5 - 9 July 2008

UNIVERSITÉ DE SHERBROOKE

Réseau québécois de calcul de haute performance

NSERC CRSNG

Menu

Part I :

Correlated Electron Systems

Part II :

Quantum Cluster Methods

Part III:

Variational Approach

Part I : Summary

- Dimension of the Hilbert space is enormous for $L > 16$
- Lanczos algorithm (or Band Lanczos) is able to diagonalize the Hamiltonian Matrix for a small systems.
- It gives the Green function

- Symmetries of the system reduce the dimension of the Hilbert space
- One can calculate the spectral function from the Green function

$$A(\mathbf{k},\omega) = -2 \lim_{\eta \to 0^+} \mathrm{Im}\, G(\mathbf{k},\omega + i\eta)$$

- and/or the density of states

$$n(\omega) = \int_{\mathbf{k}} A(\mathbf{k},\omega)$$

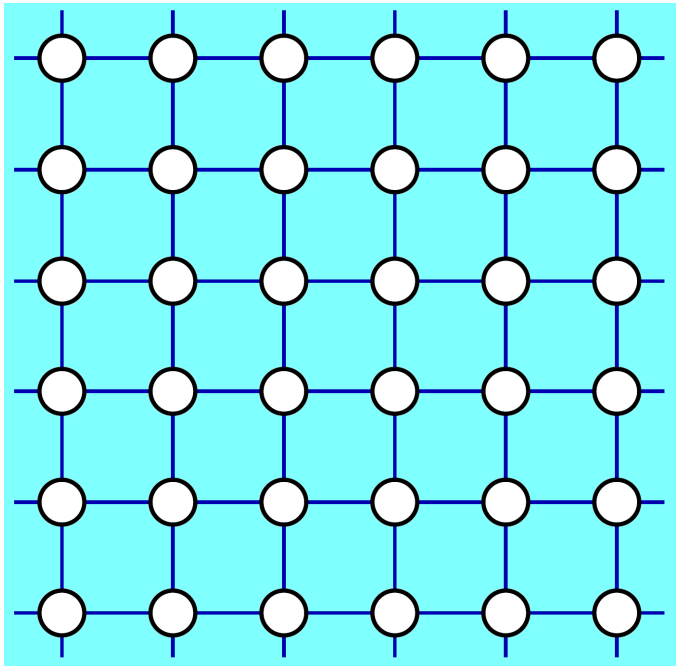
Part II

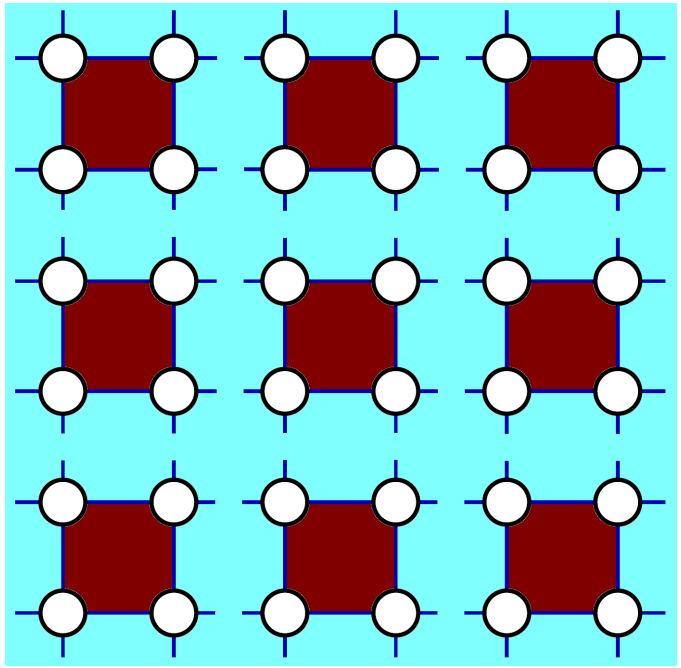
Cluster Perturbation Theory

Cluster Perturbation Theory

Goal:

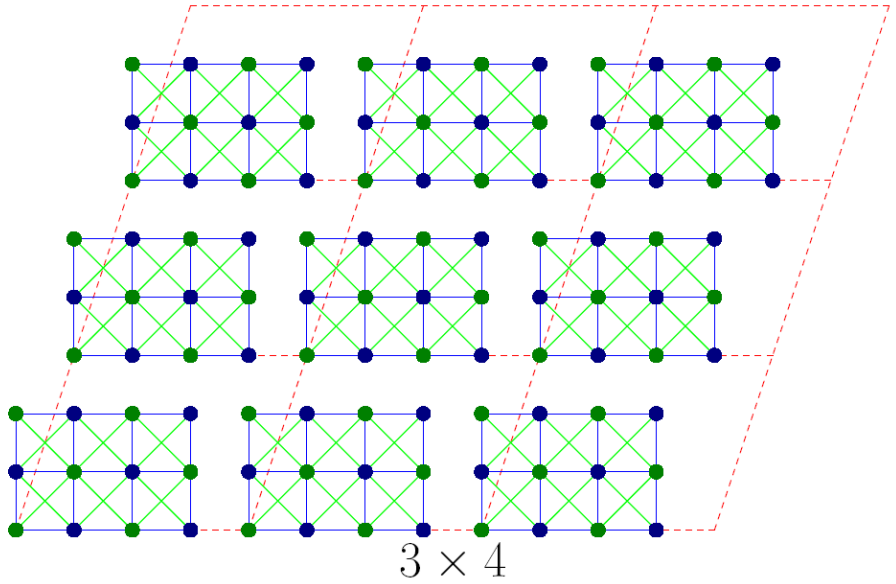
- approximate value for the Green function $G_{ij}(\omega)$ of the model.





Cluster Perturbation Theory

D. Sénéchal, et al. PRL84 2000
D. Sénéchal, et al. PRB66 2002



Basic idea:

- Tile the lattice into a superlattice of identical clusters of L sites
- Calculate the Green Function of a cluster $G'_{ij}(\omega)$ exactly (Lanczos method)
- Extract the self-energy and extend it over the lattice

Cluster Perturbation Theory

$$H = H' + V$$

H	lattice Hamiltonian
H'	cluster Hamiltonian
V	inter-cluster hopping terms

$$\mathsf{t} = \mathsf{t}' + \mathsf{V}$$

t	hopping matrix
t'	cluster hopping matrix
V	inter-cluster hopping

C. Gros and R. Valenti, Phys. Rev. B 48, 418 (1993)
D. Sénéchal, D. Perez, and M. Pioro-Ladriere. Phys. Rev. Lett. 84, 522 (2000)

Cluster Perturbation Theory

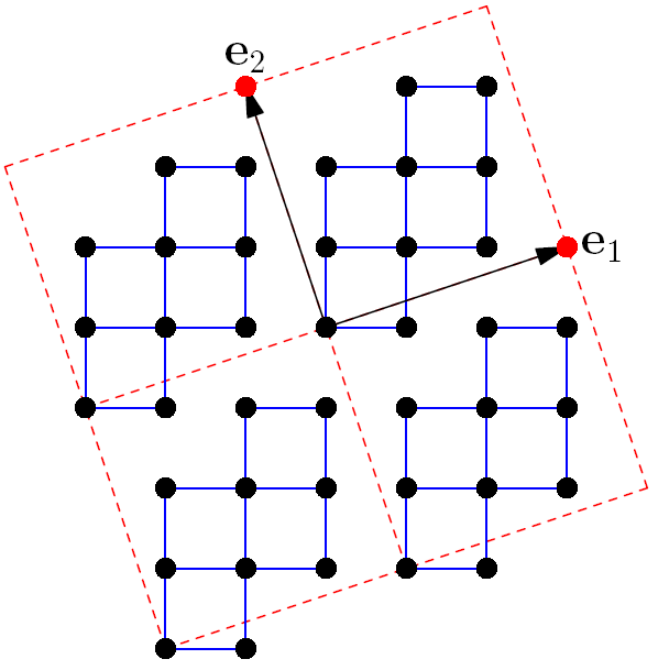
- V is treated at *lowest order in Perturbation theory*
- At this order, the Green function is:

$$\mathsf{G}^{-1}(\omega) = \mathsf{G}'^{-1}(\omega) - \mathsf{V}$$

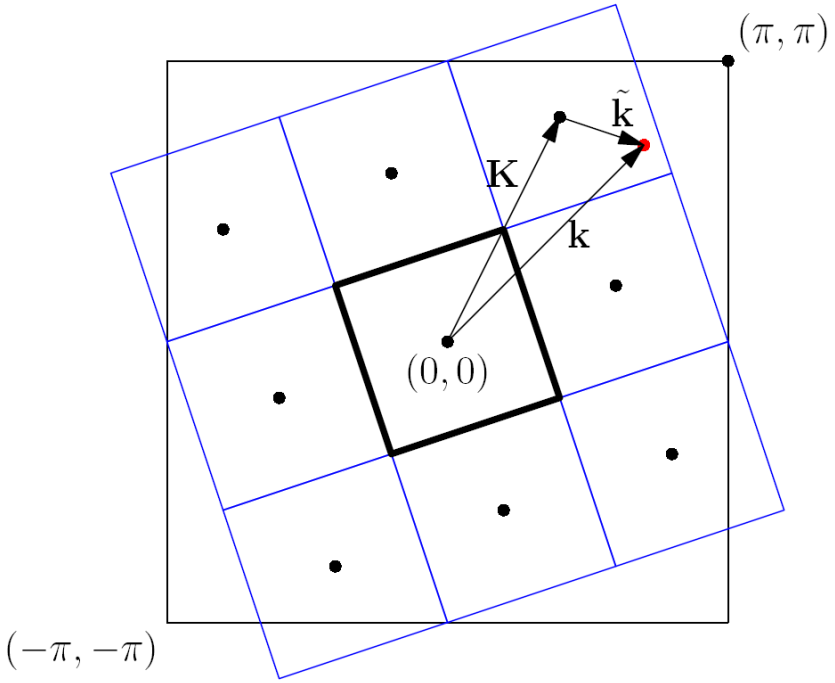
G' : cluster Green function

C. Gros and R. Valenti, Phys. Rev. B 48, 418 (1993)
D. Sénéchal, D. Perez, and M. Pioro-Ladriere. Phys. Rev. Lett. 84, 522 (2000)

Cluster Perturbation Theory



Cluster in real space



Reduced Brillouin zone

Cluster Perturbation Theory

$i; j$: lattice site index

$m; n$: lattice site index

$a; b$: cluster site index

$\mathbf{k}$: full wavevector

$\tilde{\mathbf{k}}$: redcued wavevector

$\mathbf{K}$: cluster wavevector

$$f_j = \sum_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_j} f(\mathbf{k}) \qquad f(\mathbf{k}) = \frac{1}{N}\sum_{j} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}_j} f_j$$

$$f_m = \sum_{\tilde{\mathbf{k}}} \mathrm{e}^{i\tilde{\mathbf{k}}\cdot\mathbf{r}_m} f(\tilde{\mathbf{k}}) \qquad f(\tilde{\mathbf{k}}) = \frac{L}{N}\sum_{m} \mathrm{e}^{-i\tilde{\mathbf{k}}\cdot\mathbf{r}_m} f_m$$

$$f_a = \frac{1}{\sqrt{L}}\sum_{\mathbf{K}} \mathrm{e}^{i\mathbf{K}\cdot\mathbf{r}_a} f_{\mathbf{K}} \qquad f_{\mathbf{K}} = \frac{1}{\sqrt{L}}\sum_{a} \mathrm{e}^{-i\mathbf{K}\cdot\mathbf{r}_a} f_a$$

Cluster Perturbation Theory

G' is the cluster Green function, and
G_0 is the lattice free Green function

$$G'^{-1} = \omega - t' - \Sigma$$

$$G_0^{-1} = \omega - t = \omega - (t' + V)$$

$$= \omega - t' - V$$

We had:

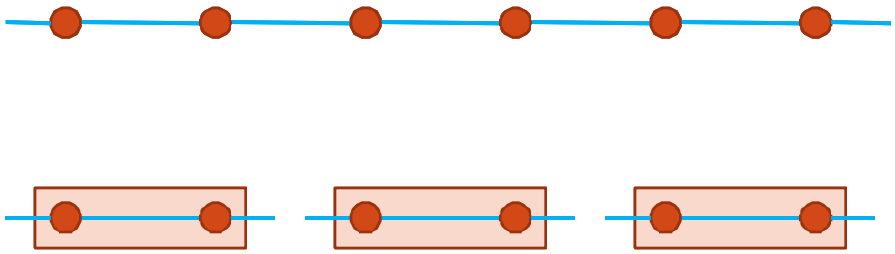
$$G^{-1}(\omega) = G'^{-1}(\omega) - V$$

Thus : lattice self-energy is approximated as the cluster self-energy

$$G^{-1}(\tilde{\mathbf{k}}, \omega) = {G_0}^{-1}(\tilde{\mathbf{k}}, \omega) - \Sigma(\omega)$$

Cluster Perturbation Theory

Example : 2-site cluster in 1 dimension:



$$\mathsf{t}' = -t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \mathsf{V}(\tilde{k}) = -t \begin{pmatrix} 0 & e^{-2i\tilde{k}} \\ e^{2i\tilde{k}} & 0 \end{pmatrix}$$

CPT : Relation with spectral function

$$A(\mathbf{k},\omega) = -2 \lim_{\eta \to 0^+} \mathrm{Im}\, G(\mathbf{k},\omega + i\eta)$$

- Probability that an electron of wavevector $\mathbf{k}$ injected into ($\omega > 0$) or ejected from ($\omega < 0$) the system have energy $\hbar\omega$
- The electron spectral function can be probed by ARPES

The density of states is simply :

$$n(\omega) = \int_{\mathbf{k}} A(\mathbf{k},\omega)$$

CPT : Relation with spectral function

Lehmann representation:

$$
\begin{aligned}
G_{\alpha\beta}(\omega) &= \sum_m \langle \Omega | c_\alpha | m \rangle \frac{1}{\omega - E_m + E_0} \langle m | c_\beta^\dagger | \Omega \rangle \\
&\quad + \sum_n \langle \Omega | c_\beta^\dagger | n \rangle \frac{1}{\omega + E_n - E_0} \langle n | c_\alpha | \Omega \rangle
\end{aligned}
$$

knowing that $\lim_{\eta \to 0^+} \mathrm{Im} \frac{1}{\omega + i\eta} = \lim_{\eta \to 0^+} \mathrm{Im} \frac{\eta}{\omega^2 + \eta^2} = -\pi \delta(\omega)$

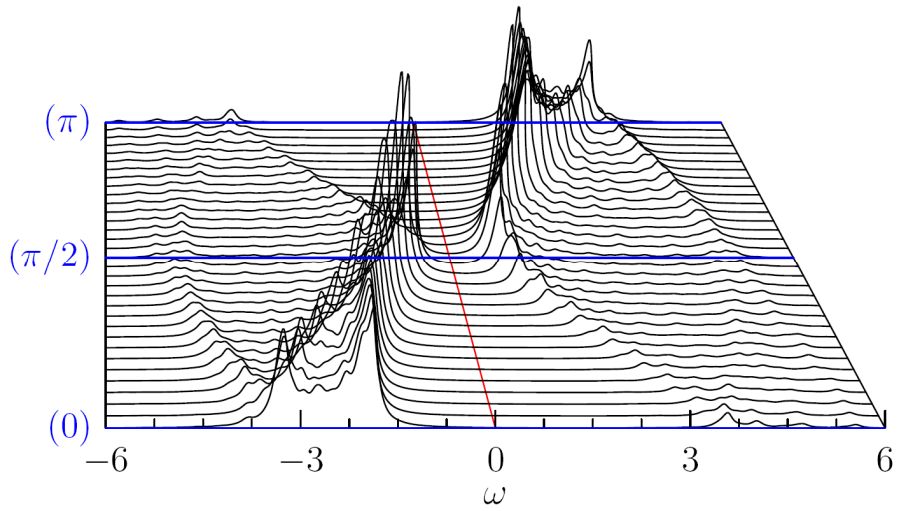
$$
\begin{aligned}
A(\mathbf{k}, \omega) &= \sum_m |\langle m | c_\mathbf{k}^\dagger | \Omega \rangle|^2 2\pi \delta(\omega - E_m + E_0) \\
&\quad + \sum_n |\langle n | c_\mathbf{k} | \Omega \rangle|^2 2\pi \delta(\omega + E_n - E_0)
\end{aligned}
$$

Cluster Perturbation Theory

CPT breaks translation invariance (open bc), which needs to be restored.

Periodizing the Green function:

$$G_{\rm cpt}(\mathbf{k},\omega) = \frac{1}{L}\sum_{a,b} \mathrm{e}^{-i\mathbf{k}\cdot(\mathbf{r}_a-\mathbf{r}_b)} G_{ab}(\tilde{\mathbf{k}},\omega)$$



Cluster Perturbation Theory

Summary :

- Exact at $U = 0$
- Exact at $t_{ij} = 0$
- Exact short-range correlations
- Allows all values of the wavevector
- But : No long-range order
- Controlled by the size of the cluster

The self-energy functional approach

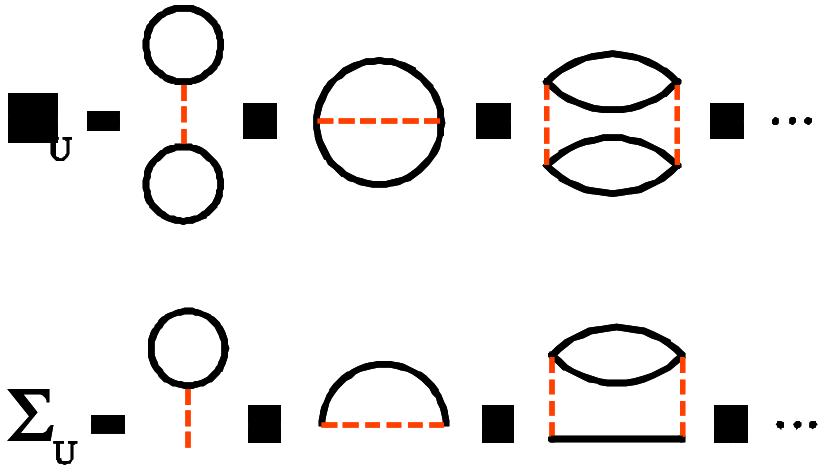
Self-energy Functional Approach

Variational principle for the Green function:

$$\Omega_t[G] = \Phi[G] - \mathrm{Tr}\left((G_{0t}^{-1} - G^{-1})G\right) + \mathrm{Tr}\,\ln(-G)$$

. . . with the property $\dfrac{\delta\Phi[G]}{\delta G} = \Sigma$

Where $\phi[G]$ is the Luttinger-Ward functional:



Luttinger, Ward (1963)

Self-energy Functional Approach

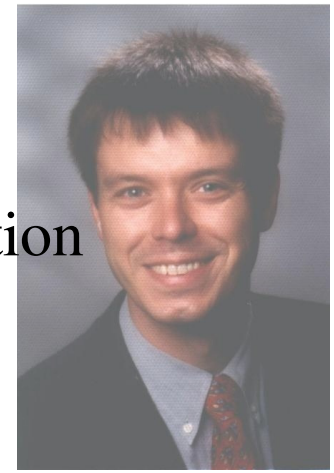
Here, Tr means a sum over frequencies, site indices (or wavevectors) and spin/band indices.

The functional is stationary at the physical Green function (Euler eq.):

$$\frac{\delta \Omega_t[G]}{\delta G} = \Sigma - G_{0t}^{-1} + G^{-1} = 0$$

- Approximation schemes:
  - Type I : Simplify the Euler equation
  - Type II : Approximate the functional (Hartree-Fock, FLEX)
  - Type III : Restrict the variational space, but keep the functional exact

Self-energy Functional Approach



Potthoff : Use the self-energy rather than the Green function

$$\Omega_t[\Sigma] \quad = \quad F[\Sigma] - \ \mathrm{Tr}\ \ln(-\mathsf{G}_{0t}^{-1} + \Sigma)$$

F is the Legendre transform of ϕ

$$F[\Sigma] \quad = \quad \Phi[\mathsf{G}] - \ \mathrm{Tr}\,(\Sigma\mathsf{G})$$

$$\frac{\delta F[\Sigma]}{\delta \Sigma} = \frac{\delta \Phi[\mathsf{G}]}{\delta \mathsf{G}} \frac{\delta \mathsf{G}[\Sigma]}{\delta \Sigma} - \Sigma \frac{\delta \mathsf{G}[\Sigma]}{\delta \Sigma} - \mathsf{G} = -\mathsf{G}$$

M. Potthoff, Eur. Phys. J. B , 2003

Self-energy Functional Approach

New Euler equation:

$$\frac{\delta \Omega_t[\Sigma]}{\delta \Sigma} = -G + (G_{0t}^{-1} - \Sigma)^{-1} = 0$$

At the physical self-energy $\Omega_t[\Sigma]$ is the thermodynamic grand potential

SFA : The Reference System

- To evaluate F, use its universal character : its functional form depends only on the interaction.
- Introduce a reference system H', which differs from H by one-body terms only (example : the cluster Hamiltonian)
- Suppose H' can be solved exactly.

Then, at the physical self-energy Σ of H' :

$$\Omega' = F[\Sigma] - \mathrm{Tr}\ \ln(-\mathsf{G}')$$

SFA : The Reference System

by eliminating F :

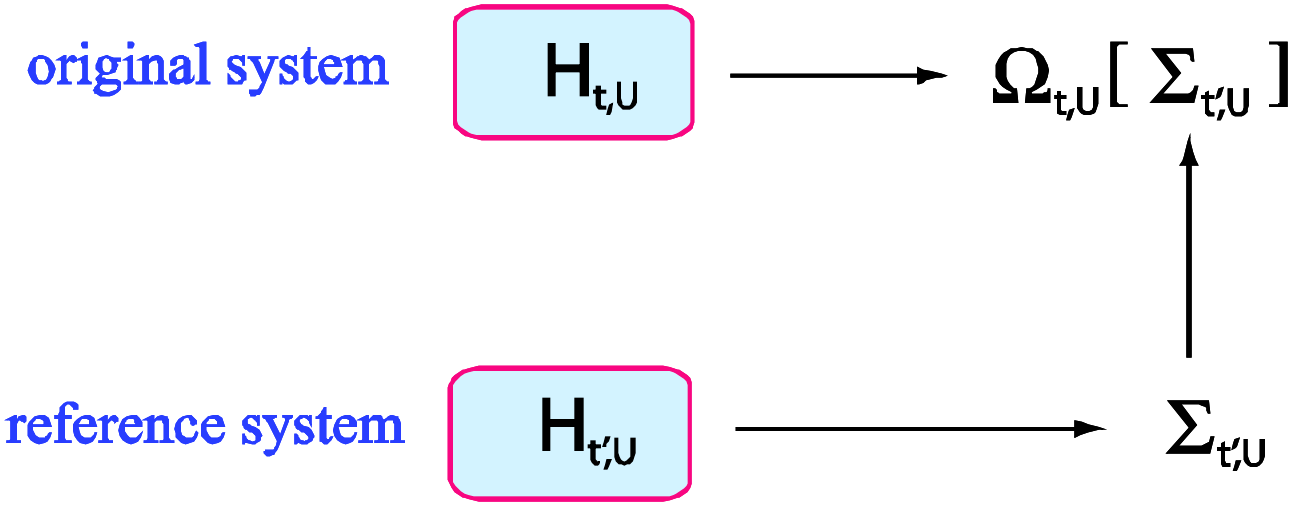
$$\begin{aligned}\Omega_t[\Sigma] &= \Omega' + \mathrm{Tr}\,\ln(-G') - \mathrm{Tr}\,\ln(-G_{0t}^{-1} + \Sigma) \\ &= \Omega' + \mathrm{Tr}\,\ln(-G') - \mathrm{Tr}\,\ln(-G)\end{aligned}$$

$$\Omega_t[\Sigma] = \Omega' - \mathrm{Tr}\,\ln(1 - VG')$$

- The sum over frequencies is to be performed over Matsubara frequencies (or an integral along the imaginary axis at $T = 0$).
- The variation is done over one-body parameters of the cluster Hamiltonian H
- In particular, the Weiss field M is to be varied until is stationary

Self-energy Functional Approach

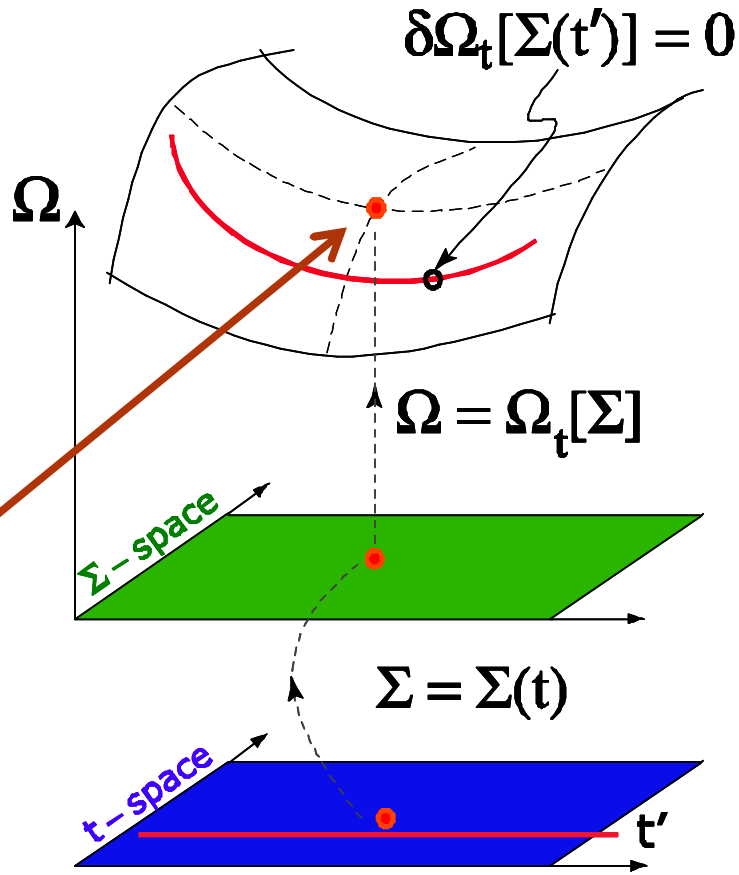
Summary :



SFA : The Reference System

SEF: $\Omega[\Sigma]$ is stationary at physical self-energy

$$\left.\frac{\delta\Omega[\Sigma]}{\delta\Sigma}\right|_{\Sigma_{physical}} = 0$$



- Therefore, $\Omega[\Sigma]$ can be written as the direct function of the physical variables h:

$$\Sigma = \Sigma(h)$$

$$\Omega = \Omega[\Sigma(h)] = \Omega(h)$$

To be continued ...