Functionals in many particle systems   Chapter 8

- Concise formulation of various useful approximation
  DFT, DMFT, GW, ...
- "Conserving functionals" conserve energy, momentum, particle number
  an provide "best" approximations.
- stationary functionals allow robust solution even when
  implementation is approximate

Most famous Functional theory is DFT. (chapter 4.3 in Z.M. book)

It is indirect approach in solving the many body problem, in which charge density $\rho(\vec{r})$ is the central quantity to be determined.

Total energy (at $T=0$) can be expressed by:

$$E = \langle\Psi|H|\Psi\rangle = \langle\Psi|T + V_{ee} + V_{nuc}|\Psi\rangle = \langle\Psi|\underbrace{T+V_{ee}}_{\text{universal because it has explicit form}}|\Psi\rangle + \underbrace{\int d^3r\,\rho(\vec{r})\,V_{nuc}(\vec{r})}_{\text{non-universal depends on the "material"}}$$

$$T = \sum_i -\frac{\nabla_i^2}{2m_i}\ ;\quad V = \frac{1}{2}\sum_{i\neq j} V_c(\vec{r}_i - \vec{r}_j)$$

- Hohenberg and Kohn proved that H is a unique functional of the ground state charge density $\rho(\vec{r})$. In another words, there can not be two potentials $V^{(1)}_{nuc}(\vec{r})$ and $V^{(2)}_{nuc}(\vec{r})$ giving rise to the same ground state electron density $\rho(\vec{r})$. Hence if we know $\rho(\vec{r}) \Rightarrow$ we know $V_{nuc}(\vec{r}) \Rightarrow$ we know H.

If we know $H \Rightarrow$ there is unique ground state $|\Psi_0\rangle$ and corresponding $E = \langle\Psi_0|H|\Psi_0\rangle$ is uniquely determined from $\rho(\vec{r})$. Also all ground state properties are uniquely determined by $\rho(\vec{r})$.

Proof that H is unique functional of $\rho(\vec{r})$: Assume there exist two potentials $V_{nuc}^{(1)}(\vec{r})$ and $V_{nuc}^{(2)}(\vec{r})$ differing by more than a constant, and giving rise to the same g.s. density $\rho(\vec{r})$. We have

$$(T+V_{ee}+V_{nuc}^{(1)})|\psi^{(1)}\rangle = E^{(1)}|\psi^{(1)}\rangle$$
$$(T+V_{ee}+V_{nuc}^{(2)}|\psi^{(2)}\rangle = E^{(2)}|\psi^{(2)}\rangle$$

$|\psi^{(1)}\rangle$ and $|\psi^{(2)}\rangle$ are different. Then:

$$E^{(1)} = \langle\psi^{(1)}|H^{(1)}|\psi^{(1)}\rangle < \langle\psi^{(2)}|H^{(1)}|\psi^{(2)}\rangle$$

because of variational principle, any $|\psi^{(2)}\rangle$, which is not g.s. should give strictly higher energy.

We assumed $H^{(1)} = H^{(2)} + V_{nuc}^{(2)} - V_{nuc}^{(1)}$ therefore:

$$E^{(1)} = \langle\psi^{(1)}|H^{(1)}|\psi^{(1)}\rangle < \underbrace{\langle\psi^{(2)}|H^{(2)}|\psi^{(2)}\rangle}_{E^{(2)}} + \underbrace{\langle\psi^{(2)}|V_{nuc}^{(2)}-V_{nuc}^{(1)}|\psi_2\rangle}_{\int[V_{nuc}^{(2)}(\vec{r})-V_{nuc}^{(1)}(\vec{r})]\rho(\vec{r})d^3r}$$

exchange $(1)\Leftrightarrow(2)$

$$E^{(2)} = \langle\psi^{(2)}|H^{(2)}|\psi^{(2)}\rangle < E^{(1)} + \int[V_{nuc}^{(1)}(\vec{r})-V_{nuc}^{(2)}(\vec{r})]\rho(\vec{r})d^3r$$

sum the two equations:

$$E^{(1)}+E^{(2)} < E^{(2)}+E^{(1)}$$ which is absurd $\Rightarrow$ conclusion $V_{nuc}^{(1)}-V_{nuc}^{(2)}=0$ or constant.

We just proved that if we are given ground state density $\rho(\vec{r})$ we can uniquely determine $V_{nuc}(\vec{r})$ and hence H.
Since we have unique H, we could in principle find unique $|\psi^0\rangle$ and any ground state property.

Note: H.K. theorem breaks for degenerate ground states. In this case $|\psi^{(2)}\rangle$ and $|\psi^{(1)}\rangle$ have the same energy, but different density. Example "Mott insulator".

- H.K. also proved that $E[\rho]$ reaches minimum in the exact ground state density $\rho(\vec{r})$.

Proof: If $|\psi^{(2)}\rangle$ gives rise to density $\rho^{(2)}(\vec{r})$, which is different from g.s., we have

$$E[\rho] = \langle\psi^{(1)}|H|\psi^{(1)}\rangle < \langle\psi^{(2)}|H|\psi^{(2)}\rangle$$ because of the variational principle because $|\psi^{(2)}\rangle$ is not g.s. wave function, while $|\psi^{(1)}\rangle$ is.

Second step: Kohn-Sham auxiliary non-interacting system:

The exact g.s. density is represented in terms of some non-interacting set of orbitals, i.e., $\rho(\vec{r}) = \sum_{i\in occ} \psi_i^*(\vec{r})\, \psi_i(\vec{r})$

The kinetic energy is then expressed by $T_{ip}[\rho] = \sum_{i\in occ} \int \psi_i^*(\vec{r}) \left(-\frac{\nabla^2}{2m}\right) \psi_i(\vec{r})\, d^3r$

Therefore

$$E[\rho] = \sum_{i\in occ} \int \psi_i^*(\vec{r}) \left(-\frac{\nabla^2}{2m} + V_{nuc}(\vec{r})\right) \psi_i(\vec{r}) + E^H[\rho] + E^{xc}[\rho]$$

where $E^H[\rho] = \frac{1}{2} \iint \frac{\rho(\vec{r})\, \rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\, d^3r\, d^3r'$ is the Hartree term.

$E^{xc}[\rho]$ is unknown functional. It's exact expression is

$$E^{xc}[\rho] = \langle T \rangle - T_{ip}[\rho] + \langle V_{ee} \rangle - E^H[\rho]$$ and is rather small

because $\langle T \rangle \approx T_{ip}[\rho]$ and $\langle V_{ee} \rangle \approx E^H[\rho]$

Moreover $E^{xc}[\rho]$ is universal functional $\Rightarrow$ can be computed in any simple interacting system. Idea: Solve the uniform electron problem and determine $E^{xc}[\rho]$ and use it in any material.

Unfortunately uniform electron gas is not solvable exactly, but we only know numerical value of $E^{xc}[\rho]$ where ρ is a constant density $\rho = n =$ constant in space.

Idea: Approximate $E^{xc}[\rho] = \int d^3r\, \rho(\vec{r})\, \varepsilon^{xc}[\rho(\vec{r})]$, i.e., to each point in space we can associate energy density $\varepsilon^{xc}[\rho(\vec{r})]$, and it's value depends on charge density at $\rho(\vec{r})$. [does not depend on $\rho(\vec{r}\,' \neq \vec{r})$].

This approximation is called "Local density approximation" LDA.

From solution of UEG we know $\varepsilon^{xc}[\rho]$ hence we can now solve DFT equations.

We are looking for the minimum of the functional $E[\rho]$ under constraint that K.S. orbitals are normalized. Hence we can perform constraint minimization:

$$\frac{\delta E}{\delta \rho} - \sum_i \varepsilon_i \left(\int \psi_i^*(\vec{r}) \psi_i(\vec{r}) d^3r - 1 \right) = 0$$

Note that $\frac{\delta}{\delta \rho}$ can be written as $\frac{\delta \psi_k^*(\vec{r})}{\delta \rho} \frac{\delta}{\delta \psi_k^*(\vec{r})}$

$$0 = \frac{\delta}{\delta \psi_k^*}\left(E[\rho] - \varepsilon_i \int \psi^* \psi\right) = \frac{\delta}{\delta \psi_k^*}\left\{\sum_{i \in occ} \int \psi_i^*(\vec{r}) \left(-\frac{\nabla^2}{2m} + V_{nuc}(\vec{r}) - \varepsilon_i\right) \psi_i(\vec{r}) + E^H[\rho] + E^{xc}[\rho]\right\}$$

$$= \left(-\frac{\nabla^2}{2m} + V_{nuc}(\vec{r}) - \varepsilon_k\right)\psi_k(\vec{r}) + \left(\frac{\delta E^H[\rho]}{\delta \rho} + \frac{\delta E^{xc}[\rho]}{\delta \rho}\right) \frac{\delta \rho}{\delta \psi_k^*}$$

Define $\frac{\delta E^H[\rho]}{\delta \rho} \equiv V^H[\rho]$ $\qquad V^H[\rho] = \int \frac{\rho(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|} d^3r'$

$\frac{\delta E^{xc}[\rho]}{\delta \rho} = V^{xc}[\rho]$ $\qquad V^{xc}[\rho] = \varepsilon^{xc}(\rho) + \rho \cdot \frac{\delta \varepsilon^{xc}}{\delta \rho}$

hence:

$$\left(-\frac{\nabla^2}{2m} + V_{nuc}(\vec{r}) + V^H_{(\vec{r})} + V^{xc}_{(\vec{r})} - \varepsilon_k\right) \psi_k(\vec{r}) = 0$$

This is Schroedinger equation for a non-interacting system. Note that DFT is "interacting theory" because $V^{xc}[\rho]$ has to be computed self-consistently. All correlations are hidden in this $V^{xc}(\vec{r})$ function.

Note that this is actually a Dyson equation for the Kohn-Sham green's function

$$\left.\begin{aligned} (\mathcal{G}^0)^{-1} &\equiv \omega + \mu + \frac{\nabla^2}{2m} - V_{nuc}(\vec{r}) \\ \Sigma(\vec{r}, \vec{r}\,') &= [V^H(\vec{r}) + V^{xc}(\vec{r})]\, \delta(\vec{r} - \vec{r}\,') \\ \mathcal{G}(\vec{r}, \vec{r}\,') &= \sum_k \psi_k(\vec{r}) \frac{1}{\omega + \mu - \varepsilon_k} \psi_k^*(\vec{r}\,') \end{aligned}\right\}$$

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

$$\sum_k \Big[\omega + \mu + \underbrace{\frac{\nabla^2}{2m} - V_{nuc}(\vec{r}) - V^H - V^{xc}}_{-\varepsilon_k}\Big] \psi_k(\vec{r}) \frac{1}{\omega + \mu - \varepsilon_k} \psi_k^*(\vec{r}\,')$$

$$\sum_k \psi_k(\vec{r}) \frac{\omega + \mu - \varepsilon_k}{\omega + \mu - \varepsilon_k} \psi_k^*(\vec{r}\,') = \delta(\vec{r} - \vec{r}\,')$$

because ψ_k are a complete basis.

We proved that $(\mathcal{G}_0^{-1} - \Sigma)\mathcal{G} = 1 \implies \mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \Sigma$ hence this equation defines the Dyson equation for $\mathcal{G} = \sum_k \psi_k(\vec{r}) \frac{1}{\omega + \mu - \varepsilon_k} \psi_k^*(\vec{r})$

One can define a functional of this green's function $\mathcal{G}(\vec{r}, \vec{r}')$, which gives identical equations to DFT, but it becomes then an approximation for excitations, not just the ground state properties.

The functional is:

$$\Gamma[\mathcal{G}] = \mathrm{Tr}\ln(-\mathcal{G}) - \mathrm{Tr}((\mathcal{G}_0^{-1} - \mathcal{G}^{-1})\mathcal{G}) + E^H[\rho] + E^{xc}[\rho]$$

where $\rho(\vec{r}) = \mathcal{G}(\vec{r}\tau, \vec{r}'\tau')\,\delta(\vec{r}-\vec{r}')\,\delta(\tau-\tau')$

Optimizing the functional $\frac{\delta\Gamma}{\delta\mathcal{G}} = 0$ gives

$$0 = \frac{\delta\Gamma}{\delta\mathcal{G}} = \mathcal{G}^{-1} - \mathcal{G}_0^{-1} + \frac{\delta\rho}{\delta\mathcal{G}} \frac{\delta}{\delta\rho}\left(E^H[\rho] + E^{xc}[\rho]\right)$$

$$= \mathcal{G}^{-1} - \mathcal{G}_0^{-1} + (V^H + V^{xc})\,\delta(\vec{r}-\vec{r}')\,\delta(\tau-\tau')$$

hence $\Sigma(\vec{r}\tau, \vec{r}'\tau') = (V^H(\vec{r}) + V^{xc}(\vec{r}))\,\delta(\vec{r}-\vec{r}')\,\delta(\tau-\tau')$ which exactly shows that $\Gamma[\mathcal{G}]$ delivers the same DFT equations and the same solution.

But here we get $\mathcal{G}(\vec{r}, \tau)$ as approximation to the single particle green's function (band structure), not just the ground state properties.

However, even if the exact $E^{xc}[\rho]$ is known, this functional is still an approximation for the spectra. We will show later what is the exact $E^{xc}[\mathcal{G}]$ later in this chapter, and we will contrast it with $E^{xc}[\rho]$.

Most often used approximations include GGA and meta-GGA's, hybrids, DFT+U, DFT+DMFT, ...

- GGA: The functional is parametrized with more freedom, and $\varepsilon^{xc}(\vec{r})$ depends on $\rho(\vec{r})$ as well as $\nabla\rho(\vec{r})$, i.e.,

$$E^{xc}[\rho] = \int \varepsilon^{xc}[\rho(\vec{r}), \nabla\rho(\vec{r})]\, \rho(\vec{r})\, d^3r$$

A few conservation-laws and exact relation are used to determine unknown coefficients.

- meta-GGA: $\varepsilon^{xc}(\vec{r})$ is allowed to depend on the kinetic energy part $\varepsilon^{xc}(\rho(\vec{r}), \nabla^2\psi_k(\vec{r}))$

- DFT+U: Functional depends on the density matrix of the "correlated orbitals" of a heavy atom:

$$E^{xc}[\rho, N^{\vec{R}}_{LL'}]$$

where $N^{\vec{R}}_{LL'} = \sum_{k \in occ.} \int d^3r\, d^3r'\, \psi^*_k(\vec{r})\, Y_L(\widehat{r-R})\, \delta(r-r')\, Y_{L'}(\widehat{r'-R})\, \psi_k(\vec{r}')$

One obtains an Anderson-like impurity model, which is solved by the mean-field.

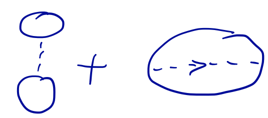
- DFT+DMFT: Functional depends on the single particle Green's function of the "correlated orbitals" or "correlated clusters".

$$E^{xc}[\rho, \hat{P}\mathcal{G}(\vec{r}, \vec{r}')]$$

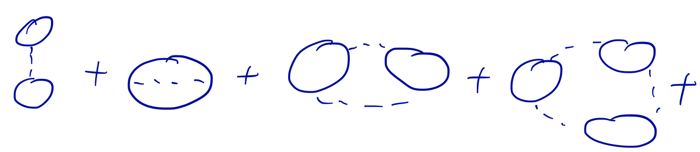
$$\hat{P}\mathcal{G}(\vec{r}, \vec{r}') = \sum_{\alpha,\beta} \phi_\alpha(\vec{r})\, \mathcal{G}_{\alpha\beta}(\omega)\, \phi^*_\beta(\vec{r}')$$ where α, β are the important degrees of freedom treated by DMFT. The generalized Anderson impurity model needs to be solved numerically by an impurity solver. A true many body problem remains to be solved.

Back to search for <u>better functionals</u>

- DFT probably is the most succesful functional, and is a functional of $\rho(\vec{r})$, therefore by the construction can give only ground state properties of the system.
  No excitation spectra available.

- Functionals of the Green's function can give the ground state, as well as the single particle excitation spectra. They can be defined by the Feynman diagrammatic technique.
  The simplest is the Hartree-Fock theory: $\Phi =$ 

  Hartree Fock

  or GW: $\Phi =$ 

- Exact functional can be expressed in terms of Feynman diagrams and is known. But difficult to evaluate. In principle can give an exact solution to the many body problem.

Generating stationary functionals of physical observables

We will borrow the concept from statistical physics. We add the source term, and then perform the Legendre transform to obtain a stationary functional at constant value of the physical observable.

Example 1: Stationary functional at constant density is the free energy functional. If the particle number is not conserved, we work with Gibbs free energy (if this context it means in the presence of the source field $\mu \hat{N}$).

- Source field $H \to H - \mu \hat{N}$ where $\mu \hat{N}$ is the source field
- The free energy in the presence of the source term is the Gibbs free energy

$$\Omega[\mu] = F[N] - \mu N$$

— Legendre transform to eliminate the source (μ) in favor of observable N.

where

$$e^{-\beta \Omega[\mu]} = Z = \mathrm{Tr}\left(e^{-\beta(H-\mu N)}\right)$$

Then $$\frac{\delta \Omega}{\delta \mu} = -\frac{1}{\beta}\frac{\mathrm{Tr}\left(e^{-\beta(H-\mu N)}\hat{N}\right)\beta}{Z} = -\langle \hat{N} \rangle \equiv -N$$

- The functional $F[N]$ is the Legendre transform of the Gibbs free energy and is stationary at constant particle number.

$$F[N] = \Omega[\mu] + \mu N$$

$$\delta F[N] = \delta\Omega[\mu] + \delta\mu N + \mu \delta N = -N\delta\mu + N\delta\mu + \mu\delta N = \mu \delta N$$

hence $\frac{\delta F[N]}{\delta N} = \mu$ and vanishes when source term μN is absent.

$$\left(\frac{\delta F[N]}{\delta N} = 0\right)$$

Example 2: A single particle observable $\hat{O}$.

- Source field $H-\mu N \to H-\mu N + u\hat{O}$

$$u \text{ (source)} \qquad \hat{O} \text{ (observable)}$$

- Free energy in the presence of the source term is the Gibbs free energy:

$$e^{-\beta\Omega[u]} = Z = \mathrm{Tr}\left(e^{-\beta(H-\mu N)-\beta u\hat{O}}\right)$$

$$\Omega[u] = F[\langle O\rangle] + u\langle O\rangle$$

Legendre transform to eliminate the source in favor of the observable.

Then $\dfrac{\delta\Omega}{\delta u} = +\dfrac{\mathrm{Tr}(e^{-\cdots}\cdot O)}{\beta Z}\beta = \langle O\rangle$

- The stationary functional $F[O]$ at constant observable O is

$$F[\langle O\rangle] = \Omega[u] - u\langle O\rangle$$

and small variation $\delta F[O] = \delta\Omega[u] - u\,\delta O - O\,\delta u = -u\,\delta O$

hence F is functional of O and it is stationary when u is set to zero.

$$\left.\frac{\delta F}{\delta O}\right|_{u=0} = 0$$

Example 3: Introduce spatial and time dependent source term to get functional of the Green's function G.

- Source field: $S \to S + \int dx\,dx'\,\psi^+(x)\,y(x,x')\,\psi(x')$

here x stands for $(\vec{r},\tau)$

- The Gibbs free energy in the presence of the field is

$$e^{-\beta\Omega[y]} = Z = \int D[\psi^+\psi]\,e^{-S-\int dx\,dx'\,\psi^+(x)\,y(x\,x')\,\psi(x')}$$

$$\frac{\delta\Omega}{\delta y(x',x)} = -\frac{1}{\beta}\frac{1}{Z}\int D[\psi^+\psi]\,e^{-S-\int\cdots}\,\psi^+(x')\,\psi(x) = \frac{1}{\beta}\langle\psi(x)\,\psi^+(x')\rangle = -G(x\,x')\frac{1}{\beta}$$

- The stationary functional $\Gamma[\mathcal{G}]$ at constant physical observable $\mathcal{G}$ is

$$\Gamma[\mathcal{G}] = \beta\Omega[\mathcal{J}] + Tr(\mathcal{G}\cdot\mathcal{J}) = \beta\Omega[\mathcal{J}] + \int dx\,dx'\, \mathcal{G}(x,x')\,\mathcal{J}(x',x)$$

We eliminated the source $\mathcal{J}$ in favor of the observable $\mathcal{G}$ in the functional.

The variation of Γ is:

$$\delta\Gamma[\mathcal{G}] = \beta\,\delta\Omega[\mathcal{J}] + \int dx\,dx' \left[\delta\mathcal{G}(x,x')\,\mathcal{J}(x',x) + \mathcal{G}(x,x')\,\delta\mathcal{J}(x',x)\right]$$

$$\beta\,\delta\Omega[\mathcal{J}] = \frac{1}{\beta}\iint\left(-\mathcal{G}(x,x')\,\delta\mathcal{J}(x',x)\right)dx\,dx'$$

hence $\delta\Gamma[\mathcal{G}] = Tr(\mathcal{J}\,\delta\mathcal{G})$

and $\left.\frac{\delta\Gamma[\mathcal{G}]}{\delta\mathcal{G}}\right|_{\mathcal{J}=0} = 0$

Γ is a functional of $\mathcal{G}$! At $\mathcal{J}=0$ is stationary.
At $\mathcal{J}=0$ $\Gamma[\mathcal{G}]$ has a value of free energy.
The later is clear from the fact that at $\Omega[\mathcal{J}=0] = F = \frac{1}{\beta}\Gamma[\mathcal{G}]\big|_{\mathcal{J}=0}$.

Note on higher order correlation functions

Higher order derivatives of Ω can give two-particle correlation function or free particle correlation functions...
If evaluated through derivative, they obey conservation laws.

$$\frac{\delta^2\Omega}{\delta\mathcal{J}(x_1,x_1')\,\delta\mathcal{J}(x_2,x_2')} = -\frac{\delta G(x_2',x_2)}{\delta\mathcal{J}(x_1,x_1')} = \frac{1}{\beta}\frac{\delta}{\delta\mathcal{J}(x_1,x_1')}\left(\frac{1}{Z[\mathcal{J}]}\int D[\psi^+\psi]\, e^{-S-\int dx\,dx'\,\psi^+(x)\,\mathcal{J}(x,x')\,\psi(x')}\,\psi(x_2')\,\psi^+(x_2)\right)$$

$$= \frac{1}{\beta}\frac{1}{Z[\mathcal{J}]}\int D[\psi^+\psi]\, e^{-S-\int dx\,dx'\,\psi^+(x)\,\mathcal{J}(x,x')\,\psi(x')}\,\psi(x_1')\,\psi^+(x_1)\,\psi(x_2')\,\psi^+(x_2)$$

$$-\frac{1}{\beta}\int D[\psi^+\psi]\, e^{-S-\cdots}\,\psi(x_2')\,\psi^+(x_2)\,\frac{1}{Z[\mathcal{J}]^2}\int D[\psi^+\psi]\, e^{-S\cdots}\,\psi(x_1')\,\psi^+(x_1)$$

$$= \langle T_\tau\psi(x_1')\,\psi^+(x_1)\,\psi(x_2')\,\psi^+(x_2)\rangle - \langle T_\tau\psi(x_2')\,\psi^+(x_2)\rangle\langle T_\tau\psi(x_1')\,\psi^+(x_1)\rangle$$

$\equiv L(1,2,1',2')$ the connected two particle correlation function

This is important to prove conservation laws.

One standard way of approximating functional $\Gamma[\mathcal{G}]$ is to use systematic expansion. (Thouless - Anderson - Palmer Eq. in spin glasses; chiral symmetry breaking in QCD)

We split the action in terms of the solvable part S^0 and the rest ΔS.

Then we write

$$S = S^0 + \lambda \Delta S + \iint \psi^\dagger y \, \psi$$

where λ is varied from 0 to 1.

At $\lambda = 0$ we have solvable problem.

At $\lambda = 1$ we have original interacting problem.

When we vary λ we keep $\mathcal{G}$ constant and add source field y so as to keep $\mathcal{G}$ fixed. At $\lambda = 1$ we set $y = 0$ so that $\mathcal{G}$ is the exact green's function of the interacting problem.

- At $\lambda = 0$, we have $S = \underbrace{\iint \psi^\dagger \mathcal{G}_0^{-1} \psi}_{S^0} + \iint \psi^\dagger y_0 \psi = \iint \psi^\dagger \underbrace{[\mathcal{G}_0^{-1} + y_0]}_{\mathcal{G}^{-1}} \psi$

The corresponding $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} + y_0$

- At $\lambda = 1$, we have $S = S^0 + \Delta S$ and we set $y_{\lambda=1} = 0$, so that $\Gamma_{\lambda=1}[\mathcal{G}]$ is the desired stationary functional.

At $\lambda = 1$ we know that $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \Sigma$, where Σ is the exact self-energy of the system.

To work at constant $\mathcal{G}$ we thus see that $y_0 = -\Sigma$

source term at $\lambda = 0$ | exact self energy

Systematic expansion could be carried out:

$$\Gamma[\mathcal{G}] = \Gamma_0[\mathcal{G}] + \lambda \Gamma_1[\mathcal{G}] + \dots$$

$$\mathcal{J}[\mathcal{G}] = \mathcal{J}_0[\mathcal{G}] + \lambda \mathcal{J}_1[\mathcal{G}] + \dots$$

We could use perturbation theory to determine order by order what is $\Gamma[\mathcal{G}]$.

Alternatively, we can split

$$\Gamma[\mathcal{G}] = \underbrace{\Gamma_0[\mathcal{G}]}_{\Gamma_0 = \Gamma(\lambda=0)} + \underbrace{\Delta\Gamma[\mathcal{G}]}_{\text{correction due to interactions.}}$$

<u>What is $\Gamma_0[\mathcal{G}]$?</u>

$\Omega_0[\mathcal{J}_0]$ can be calculated from:

$$e^{-\beta\Omega_0[\mathcal{J}_0]} = \int \mathcal{D}[\psi^\dagger,\psi]\, e^{-\iint \psi^\dagger [\mathcal{G}_0^{-1} + \mathcal{J}_0]\psi}$$ which is quadratic

and can be integrated by Gaussian integral

The result is $\int \mathcal{D}[\psi^\dagger,\psi]\, e^{-\int \psi^\dagger \mathcal{G}^{-1}\psi} = \operatorname{Det} \mathcal{G}^{-1}$ therefore

$$-\beta\Omega_0[\mathcal{J}_0] = \ln \operatorname{Det}(\mathcal{G}_0^{-1} + \mathcal{J}_0) = \operatorname{Tr}\ln \mathcal{G}^{-1} = -\operatorname{Tr}\ln\mathcal{G}$$

Indeed, for non-interacting system $\Omega_0 = -T\sum_{i\omega,\alpha} \ln(-i\omega + \varepsilon_\alpha)$ with $\mathcal{G}^{-1} = i\omega - \varepsilon_\alpha$

Then we have

$$\Gamma_0[\mathcal{G}] = \beta\Omega_0[\mathcal{J}_0] + \operatorname{Tr}(\mathcal{G}\mathcal{J}_0) = \operatorname{Tr}\ln\mathcal{G} - \operatorname{Tr}(\underset{\substack{\uparrow \\ \text{became } \mathcal{J}_0 = -\Sigma}}{\Sigma}\mathcal{G})$$

<u>Finally at $\lambda = 1$ we write:</u> $\underline{\Gamma[\mathcal{G}] = \operatorname{Tr}\ln\mathcal{G} - \operatorname{Tr}(\Sigma\mathcal{G}) + \Delta\Gamma[\mathcal{G}]}$

We will call $\Delta\Gamma[\mathcal{G}] \equiv \Phi[\mathcal{G}]$

At $\lambda=1$ we thus have: $\Gamma[\mathcal{G}] = \mathrm{Tr}\ln\mathcal{G} - \mathrm{Tr}(\Sigma\mathcal{G}) + \Phi[\mathcal{G}]$

where Φ is what is being added due to interactions.

We previously defined that at $\lambda=1$ $j=0$ (because $\mathcal{G}$ is the exact $\mathcal{G}$)

and therefore $\left.\frac{\delta\Gamma}{\delta\mathcal{G}}\right|_{\lambda=1} = 0$

Then: $\frac{\delta\Gamma}{\delta\mathcal{G}} = \underbrace{\frac{\delta}{\delta\mathcal{G}}(\mathrm{Tr}\ln\mathcal{G})}_{\mathcal{G}^{-1}} - \frac{\delta\Sigma}{\delta\mathcal{G}}\mathcal{G} - \Sigma + \frac{\delta\Phi}{\delta\mathcal{G}} = 0$

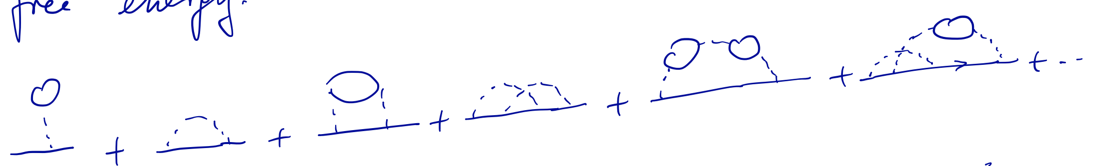
At $\lambda=1$ $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \Sigma$ and hence: $\mathcal{G}^{-2} = +\frac{\delta\Sigma}{\delta\mathcal{G}}$ therefore:

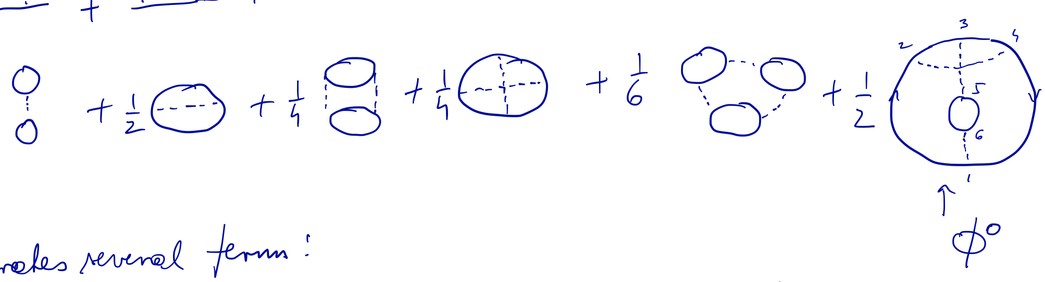
$0 = \frac{\delta\Gamma}{\delta\mathcal{G}} = \mathcal{G}^{-1} - \mathcal{G}^{-1} - \Sigma + \frac{\delta\Phi}{\delta\mathcal{G}}$ or $\boxed{\Sigma = \frac{\delta\Phi[\mathcal{G}]}{\delta\mathcal{G}}}$

We just proved that $\Phi[\mathcal{G}]$ is generating functional for Σ, i.e., Σ is obtained by cutting $\mathcal{G}$ propagators in all possible ways.

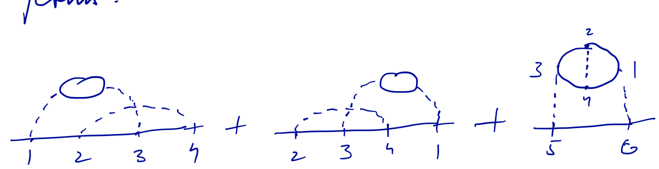
Since Σ contains all skeleton diagrams, Φ has to contain all skeleton diagrams for the free energy.

Example:

$\Sigma =$ 

$\Phi = \frac{1}{2} + \frac{1}{2} + \frac{1}{4} + \frac{1}{4} + \frac{1}{6} + \frac{1}{2}$ 

Note that $\frac{\delta\phi^0}{\delta\mathcal{G}}$ generates several terms:

$\frac{\delta\phi^0}{\delta\mathcal{G}} =$ 

Alternative derivation with power counting (Chapter 8.8, R.M.)

We start with coupling constant Integration

$$\hat{H} = \hat{H}_0 + \lambda \hat{V}_{int}$$

and $$e^{-\beta F} = Tr\left(e^{-\beta(H_0 + \lambda V_{int})}\right)$$

$$\frac{\delta F}{\delta \lambda} = +\frac{\beta}{\beta}\frac{1}{Z} Tr\left(e^{-\beta H}\, \hat{V}_{int}\right) = \langle V_{int} \rangle = \frac{1}{\lambda}\langle \lambda V_{int} \rangle$$

On page 13 we derived $\langle V_{int} \rangle = \frac{1}{2} Tr(\Sigma \mathcal{G})$ for general interacting system.

We can then write:
$$\frac{\delta F}{\delta \lambda} = \frac{1}{\lambda}\frac{1}{2} Tr(\Sigma_\lambda \mathcal{G}_\lambda)$$
where both Σ and $\mathcal{G}$ need to be evaluated for each λ.

and $$F = F(\lambda=0) + \int_0^1 \frac{1}{2\lambda} Tr(\Sigma_\lambda \mathcal{G}_\lambda)$$

Power expansion of $\Sigma_\lambda[\mathcal{G}_\lambda, v_c]$ as derived by Baym-Kadanoff.

Using Feynman diagrams technique, one can expand self energy in powers:

$\Sigma =$  $+ \cdots$

$n=1$	$n=2$	$n=3$
$\propto \lambda v_c$	$\propto \lambda^2 v_c^2$	$\propto \lambda^3 v_c^3$
$\lambda \Sigma^{(1)}[\mathcal{G}_\lambda, v_c]$	$\lambda^2 \Sigma^{(2)}[\mathcal{G}_\lambda, v_c]$	$\lambda^3 \Sigma^{(3)}[\mathcal{G}_\lambda, v_c]$

Summary: $$\Sigma = \sum_{n=1}^{\infty} \lambda^n \Sigma^{(n)}[\mathcal{G}_\lambda, v_c]$$. Note Σ is functional of $\mathcal{G}_\lambda$ and v_c.

$$\Sigma' = \sum_{m=1}^{\infty} \lambda^m \Sigma^{(m)}[\mathcal{G}_\lambda, v_c]$$

Then: $\Delta F = \frac{1}{2}\int_0^1 d\lambda \, \frac{\lambda^m}{\lambda} \mathrm{Tr}\left(\Sigma^{(m)}[\mathcal{G}_\lambda, v_c] \cdot \mathcal{G}_\lambda\right) \overset{\text{by parts}}{=} \sum_{m=1}^{\infty} \frac{\lambda^m}{2m} \mathrm{Tr}\left(\Sigma^{(m)}[\mathcal{G}_\lambda, v_c]\cdot \mathcal{G}_\lambda\right) -$

$$- \sum_{m=1}^{\infty}\int_0^1 d\lambda \, \frac{\lambda^m}{2m} \frac{d}{d\lambda} \mathrm{Tr}\left(\Sigma^{(m)}[\mathcal{G}_\lambda, v_c]\cdot \mathcal{G}_\lambda\right)$$

by parts

$dv = d\lambda \, \frac{\lambda^{m-1}}{2}$ $\qquad u = \mathrm{Tr}(\ldots)$

$v = \frac{\lambda^m}{2m}$ $\qquad du = \frac{d}{d\lambda}\mathrm{Tr}(\ldots)$

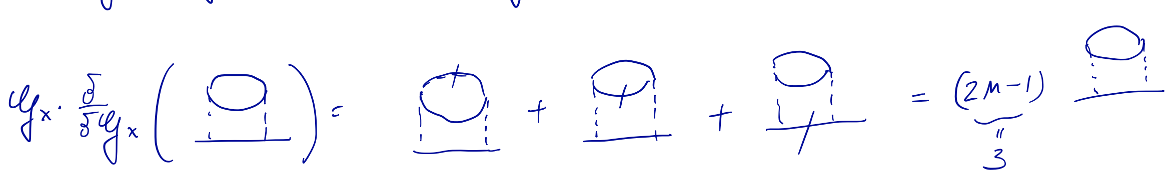
We define $\Phi[\mathcal{G}_\lambda] = \sum_{m=1}^{\infty} \frac{1}{2m} \mathrm{Tr}\left(\lambda^m \Sigma^m \cdot \mathcal{G}_\lambda\right)$ so that

$$\Delta F = \Phi[\mathcal{G}] - \sum_{m=1}^{\infty} \int_0^1 d\lambda \, \frac{\lambda^m}{2m} \mathrm{Tr}\left(\mathcal{G}_\lambda \frac{\delta \Sigma^{(m)}}{\delta \mathcal{G}^\lambda} \frac{\delta \mathcal{G}_\lambda}{\delta \lambda} + \Sigma^{(m)} \frac{\delta \mathcal{G}_\lambda}{\delta \lambda}\right)$$

Next we want to prove that $\frac{\delta \Phi}{\delta \mathcal{G}_\lambda} = \Sigma_\lambda$, i.e., Φ is the sum of skeleton free energy diagrams.

From definition follows: $\frac{\delta \Phi}{\delta \mathcal{G}_\lambda} = \sum_{m=1}^{\infty} \frac{\lambda^m}{2m}\left(\Sigma^m + \frac{\delta \Sigma^m}{\delta \mathcal{G}_\lambda}\cdot \mathcal{G}_\lambda\right) \overset{?}{=} \Sigma_\lambda$

Crucial point: $\frac{\delta \Sigma^m}{\delta \mathcal{G}_\lambda}\cdot \mathcal{G}_\lambda$ cuts one of the propagators and puts the same propagator back, hence we get back Σ^m. But there are many ways to cut, namely $(2m-1)$ ways.



It follows that: $\frac{\delta \Sigma^m}{\delta \mathcal{G}_\lambda}\cdot \mathcal{G}_\lambda = (2m-1)\Sigma^m$ and therefore $\frac{\delta \Phi}{\delta \mathcal{G}} = \sum_{m=1}^{\infty} \lambda^m \Sigma^m = \Sigma$

as promised above.

Now continue with: $\Delta F = \Phi[\mathcal{G}] - \sum_{m=1}^{\infty} \int_0^1 d\lambda \frac{\lambda^m}{2m} \mathrm{Tr}\Big(\underbrace{\underbrace{\mathcal{G}_\lambda \frac{\delta \Sigma^{(m)}}{\delta \mathcal{G}^\lambda}}_{(2m-1)\Sigma^{(m)}} \frac{\delta \mathcal{G}_\lambda}{\delta \lambda} + \Sigma^{(m)} \frac{\delta \mathcal{G}_\lambda}{\delta \lambda}}_{2m\, \Sigma^{(m)} \cdot \frac{\delta \mathcal{G}_\lambda}{\delta \lambda}} \Big)$

hence $\Delta F = \Phi[\mathcal{G}] - \sum_{m=1}^{\infty} \int_0^1 d\lambda\, \lambda^m \mathrm{Tr}\Big(\Sigma^{(m)} \frac{\delta \mathcal{G}_\lambda}{\delta \lambda}\Big)$

which is

$$\Delta F = \Phi[\mathcal{G}] - \int_0^1 d\lambda\, \mathrm{Tr}\Big(\Sigma_\lambda \frac{\delta \mathcal{G}_\lambda}{\delta \lambda}\Big)$$

once more by parts! $F = \Phi[\mathcal{G}] - \mathrm{Tr}(\Sigma_\lambda \mathcal{G}_\lambda)\Big|_0^1 + \int_0^1 d\lambda\, \mathrm{Tr}\Big(\frac{\delta \Sigma}{\delta \lambda} \mathcal{G}_\lambda\Big)$

here $\Sigma(\lambda=0) = 0$ and $\Sigma(\lambda=1) \equiv \Sigma$ hence

$$\Delta F = \Phi[\mathcal{G}] - \mathrm{Tr}(\Sigma \mathcal{G}) + \int_0^1 d\lambda\, \mathrm{Tr}\Big(\frac{\delta \Sigma}{\delta \lambda} \mathcal{G}_\lambda\Big)$$

Now we guess the last integral $R(\lambda) = -\mathrm{Tr}(\ln(1 - \mathcal{G}_0 \Sigma_\lambda))$

$$\frac{dR(\lambda)}{d\lambda} = \mathrm{Tr}\Big[(1 - \mathcal{G}_0 \Sigma_\lambda)^{-1} \mathcal{G}_0 \frac{\delta \Sigma_\lambda}{\delta \lambda}\Big]$$

$$= \mathrm{Tr}\Big[(\mathcal{G}_0^{-1} - \Sigma_\lambda)^{-1} \frac{\delta \Sigma_\lambda}{\delta \lambda}\Big] = \mathrm{Tr}\Big(\mathcal{G}_\lambda \frac{\delta \Sigma}{\delta \lambda}\Big)$$

therefore $\int_0^1 d\lambda\, \mathrm{Tr}\Big(\frac{\delta \Sigma}{\delta \lambda} \mathcal{G}_\lambda\Big) = \int_0^1 \frac{dR}{d\lambda} d\lambda = R(1) - R(0) = -\mathrm{Tr}(\ln(1 - \mathcal{G}_0 \Sigma))$

Finally $F = F_0 + \Phi[\mathcal{G}] - \mathrm{Tr}(\Sigma \mathcal{G}) - \mathrm{Tr} \ln(\mathcal{G}_0 \mathcal{G}^{-1})$

and $F = \mathrm{Tr} \ln \mathcal{G} - \mathrm{Tr}(\Sigma \mathcal{G}) + \Phi[\mathcal{G}]$

To make it stationary functional of $\mathcal{G}$ we use $\Sigma = \mathcal{G}_0^{-1} - \mathcal{G}^{-1}$ to eliminate Σ in favor of $\mathcal{G}$:

$$F[\mathcal{G}] = \mathrm{Tr} \ln \mathcal{G} - \mathrm{Tr}((\mathcal{G}_0^{-1} - \mathcal{G}^{-1}) \mathcal{G}) + \Phi[\mathcal{G}]$$

Now we can check $\frac{\delta F}{\delta \mathcal{G}} = \mathcal{G}^{-1} - \mathcal{G}_0^{-1} + \frac{\delta \Phi}{\delta \mathcal{G}} = \mathcal{G}^{-1} - \mathcal{G}_0^{-1} + \Sigma = 0$