There are two aspects to density functionals:

- The energy is expressed as a stationary functional $E(n)$ of the density $n(\vec{r}) = \left\langle \Phi_0 \left| \psi^\dagger(\vec{r}) \psi(\vec{r}) \right| \Phi_0 \right\rangle$. That can always be trivially achieved by a Legendre transform in which $H \to H + \int d^3r \; J(\vec{r}) \psi^\dagger(\vec{r}) \psi(\vec{r})$ (One could equally well contruct a stationary functional of the magnetic moment...)
- The possibility of expressing the *exact* density in terms of a Slater determinant:
$$n(\vec{r}) = \sum_{\lambda \in F} \langle \lambda | \vec{r} \rangle \langle \vec{r} | \lambda \rangle$$
The single particle orbits $|\lambda\rangle$, called Kohn-Sham orbits in this case, are calculated with a *static* (energy independent) and *local* potential:
$$[h_0 + J(\vec{r})] \langle \vec{r} | \lambda \rangle = e_\lambda \langle \vec{r} | \lambda \rangle$$

This saves a lot of complications (static potential) and computing time (local potential).

**

Do not confuse this with the possibility of expressing the energy $E(\rho) = \langle \phi | H | \phi \rangle$ of a Slater determinant as a functional of its density matrix $\rho_{ij} = \left\langle \phi \left| a_j^\dagger a_i \right| \phi \right\rangle$. The density matrix cannot be exact in this case (Hartree-Fock theory).

Consider electrons interacting with a Coulomb potential:

$$H - \mu N$$

$$= \int d^3r \; \psi^\dagger \left(\vec{r}\right) \left(h_0 - \mu\right) \psi \left(\vec{r}\right)$$

$$+ \frac{1}{2} \int d^3r_1 d^3r_2 \; \psi^\dagger \left(\vec{r}_1\right) \psi^\dagger \left(\vec{r}_2\right) \frac{e^2}{4\pi \left|\vec{r}_1 - \vec{r}_2\right|} \psi \left(\vec{r}_2\right) \psi \left(\vec{r}_1\right)$$

where $h_0 = t + u_0 \left(\vec{r}\right)$.

For nucleons interacting with $\pi, \omega, \rho, \sigma, ...$ mesons, the theory is the same, only with more terms.

After a simple bosonization the ground state energy E_0 acquires the form:

$$E_0 - \mu N_0 = -\frac{1}{\beta} \int D(\phi)\, e^{-I(\phi)}$$

The euclidian action $I(\phi)$ is a functional of the Coulomb field ϕ:

$$I(\phi) = -Tr \ln(\partial_\tau + h_0 - \mu + \phi)$$

$$+\frac{1}{2} \int d^4x_1 d^4x_2\, \phi(x_1) \left\langle x_1 \left| K^{-1} \right| x_2 \right\rangle \phi(x_2)$$

and K is the instantaneous Coulomb interaction:

$$\langle x_1 | K | x_2 \rangle = \delta(\tau_1 - \tau_2) \frac{e^2}{4\pi |\vec{r}_1 - \vec{r}_2|} \qquad (x \equiv \tau, \vec{r})$$

$=$ x_1 – – – – – – – – – – x_2

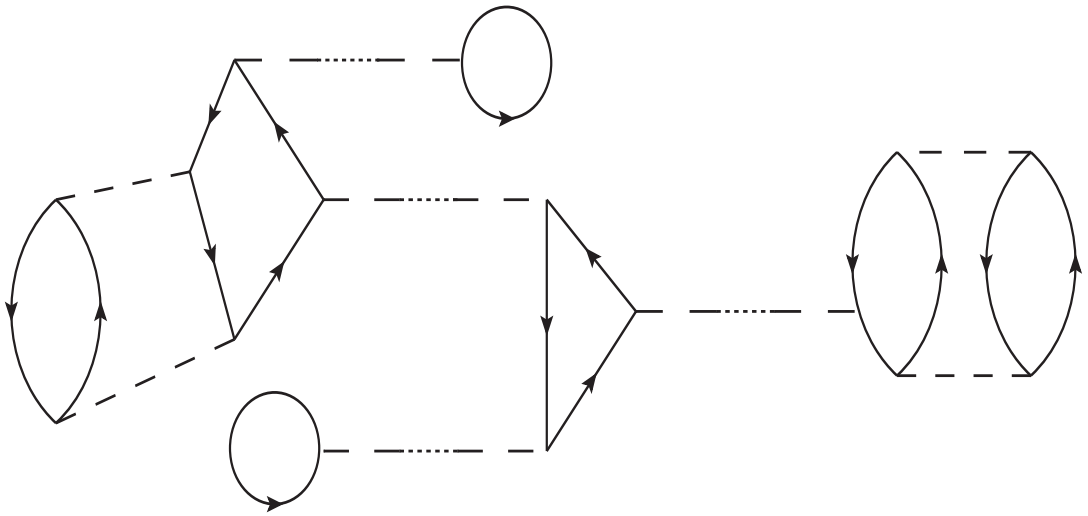
The fermion propagator is:

$$\langle x_1 | G_0 | x_2 \rangle = \left\langle x_1 \left| \frac{1}{\partial_\tau + h_0 - \mu} \right| x_2 \right\rangle$$

$=$ x_1 ⟵ x_2

The key feature is that there exists a coulomb field which couples to the density $n(\vec{r}) = \left\langle \psi^\dagger(\vec{r})\, \psi(\vec{r}) \right\rangle$ of the system.

Typical connected diagram:



The diagram has:

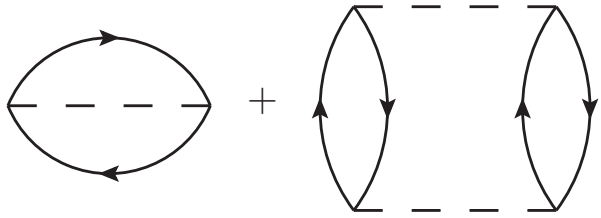
- $n_a = 4$ *articulation lines*: dashed lines such that the diagram separates into two disconnected parts when an articulation line is cut.
- $n_c = 3$ *cycles*: closed loops formed by the fermion propagators which are connected only to articulation lines.
- $n_I = 2$ *irreducible parts*: which cannot be separated into into two disconnected parts by cutting a dashed line.

$$n_I + n_c - n_a = 1$$

Let us add a local and static potential $J(\vec{r})$ to h_0. The fermion propagator becomes:

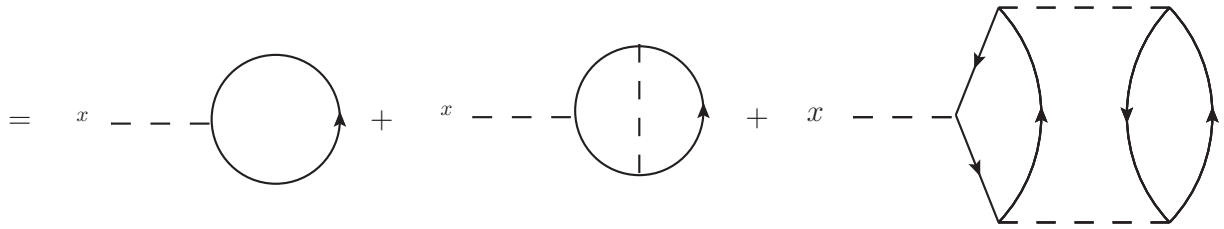
$$G(J) = \frac{1}{\partial_\tau + h_0 + J - \mu}$$

and let $\Phi(J)$ be a chosen set of irreducible diagrams calculated with the 'dressed' propagator $G(J)$:

$\Phi(J) =$  $+$

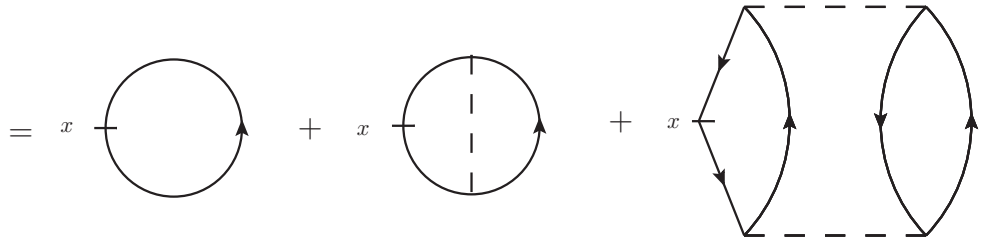
Let us choose the potential $J(\vec{r})$ to be:

$$J(x) = \int d^4y \ \langle x \left| K \right| x' \rangle \frac{\delta}{\delta J(x')} \left\{ Tr \ln G^{-1} + \Phi(J) \right\}$$



The density is then equal to:

$$n(x) = -\frac{\delta}{\delta J(x)} \left\{ Tr \ln G^{-1} + \Phi(J) \right\}$$



Note that:

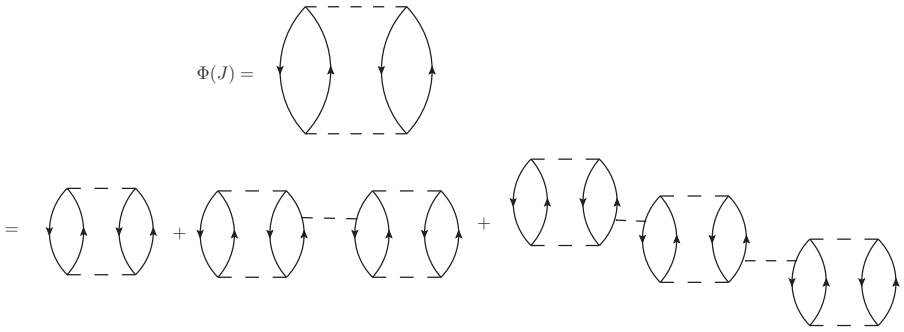
$$J(x_1) = -\int d^4y \ \langle x_1 \left| K \right| x_2 \rangle \, n(x_2)$$

$$J(\vec{r}_1) = -\int d^3r_2 \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} n(\vec{r}_2)$$

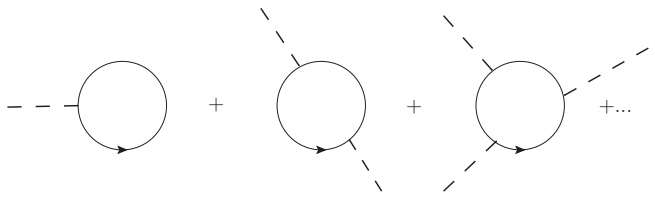
= self-consistent Coulomb potential.

The energy of the system is the sum of connected diagrams:

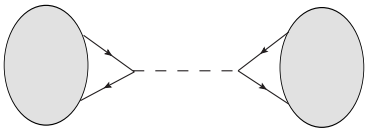
$$E_0 = -\frac{1}{\beta}\sum_{\Gamma_c}\Gamma_c$$



$$= \sum_{\Gamma_c} n_I\left(\Gamma_c\right)\Gamma_c$$



$$= \sum_{\Gamma_c} n_c\left(\Gamma_c\right)\Gamma_c = Tr\ln\left(G_0 G^{-1}\right)$$



$$= \sum_{\Gamma_c} n_a\left(\Gamma_c\right)\Gamma_c = \frac{1}{2}nKn = -\frac{1}{2}JK^{-1}J$$

Add the first two and subtract the third to get:

$$-\frac{1}{\beta}\sum_{\Gamma_c}\Gamma_c\left(n_I+n_c-n_a\right)=-\frac{1}{\beta}\sum_{\Gamma_c}\Gamma_c=E\left(J\right)$$

$$=-\frac{1}{\beta}\left\{Tr\ln G\left(J\right)+\frac{1}{2}JK^{-1}J+\Phi\left(J\right)\right\}$$

Also:

$$-\beta\frac{\delta E\left(J\right)}{\delta J\left(x\right)}=\frac{\delta}{\delta J\left(x\right)}\left(Tr\ln G\left(J\right)+\Phi\left(J\right)+K^{-1}J\right)=0$$

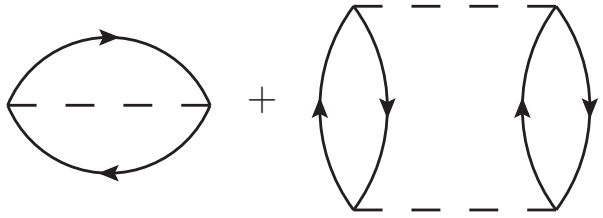
because:

$$J\left(x\right)=-K\frac{\delta}{\delta J}\left\{Tr\ln G^{-1}+\Phi\left(J\right)\right\}$$

Since $J=Kn$, $E\left(J\right)\leftrightarrow E\left(n\right)$ so that $\frac{\delta E(n)}{\delta n(x)}=0$.

Résumé:

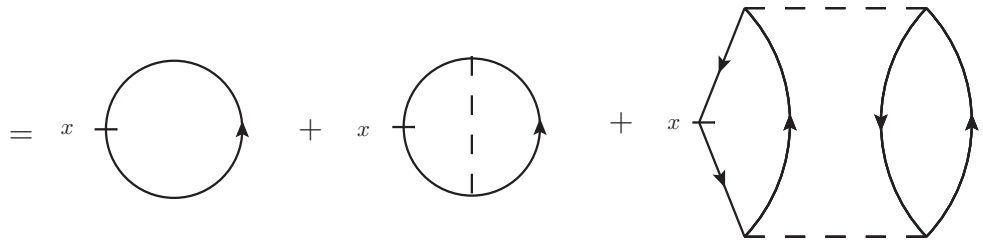
1. Make an initial guess at the potential $J(\vec{r})$.
2. Choose a set of irreducible diagrams:

$\Phi(J) =$  $+$

expressed in terms of $G^{-1} = \partial_\tau + h_0 - \mu + J(\vec{r})$.

3. Calculate the density:

$$n(x) = -\frac{\delta}{\delta J(x)} \left\{ Tr \ln G^{-1} + \Phi(J) \right\}$$

$=$ 

4. Calculate the potential $J = Kn$:

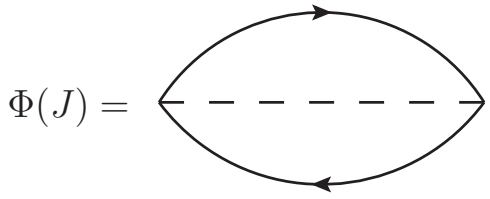
$$J(\vec{r}) = -\int d^3r' \frac{e^2}{|\vec{r} - \vec{r}'|} n(\vec{r}')$$

and return to step 2.

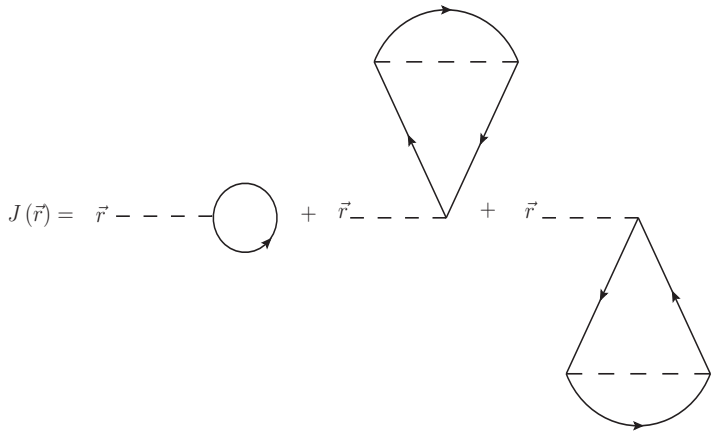
$J(\vec{r})$ is the Coulomb potential.

Simple cases.

- All one-line irreducible diagrams are neglected: $\Phi(J) = 0$. This is the Hartree approximation.
- The only irreducible diagram is:



Then:



- All one-line irreducible diagrams are included. The density and the energy are then exact.

What has this got to do with Kohn-Sham orbits? Nothing so far...

The density is equal to:

$$n(x) = -\frac{\delta}{\delta J(x)} \left\{ Tr \ln G_J^{-1} + \Phi(J) \right\}$$

$$= -\langle x | G_J | x \rangle - \frac{\delta \Phi(J)}{\delta J(x)}$$

Split the potential into two terms $J(x) = J_0(x) + J_{int}(x)$:

$$G^{-1}_{J_0+J_{int}} = \partial_\tau + h_0 - \mu + J_0 + J_{int} = G^{-1}_{J_0} + J_{int}$$

$$G^{-1}_{J_0+J_{int}} = G_{J_0} - G_{J_0} J_{int} G_{J_0+J_{int}}$$

The density becomes:

$$n(x) = -\langle x | G_{J_0} | x \rangle + \langle x | G_{J_0} J_{int} G_{J_0+J_{int}} | x \rangle - \frac{\delta \Phi(J_0 + J_{int})}{\delta J(x)}$$

Choose $J_0(x)$ such that the exact density $n(x)$ should be given by the first term:

$$n(x) = -\langle x | G_{J_0} | x \rangle = \sum_{e_\lambda < \mu} \langle \lambda | \vec{r} \rangle \langle \vec{r} | \lambda \rangle$$

$$[h_0 + J_0(\vec{r})] |\lambda\rangle = e_\lambda |\lambda\rangle$$

The $|\lambda\rangle$ are Kohn-Sham orbits. Then J_{int} is determined by:

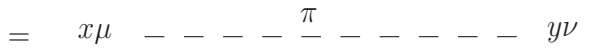
$$\langle x | G_{J_0} J_{int} G_{J_0+J_{int}} | x \rangle - \frac{\delta \Phi(J_0 + J_{int})}{\delta J(x)} = 0$$

Considerably more complicated! Except in one case...

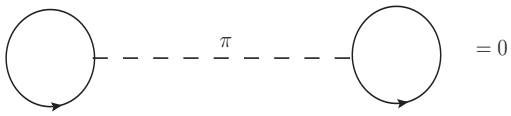
Consider the case where there are no σ nor ω mesons in the theory as in ChPT. Then $K_\phi = 0$ so that $J = K_\phi n = 0$.

Consider the case where there are only pions. The only boson propagator is:

$$\left\langle x \left| K^\pi_{\mu\nu} \right| y \right\rangle = g_A \left(\frac{1}{2f_\pi} \right)^2 \left\langle x \left| \partial_\mu \frac{1}{-\partial^2 + m_\pi^2} \partial_\nu \right| y \right\rangle$$



and (with very few exceptions) one-line irreducible diagrams vanish:



for symmetry reasons: the pion field gives rise to a potential which breaks parity. It couples to the density

$\rho_a(\vec{r}) = \left\langle \psi^\dagger(\vec{r}) \gamma_5 \tau_a \psi(\vec{r}) \right\rangle$ and not to the particle density $n(\vec{r}) = \left\langle \psi^\dagger(\vec{r}) \psi(\vec{r}) \right\rangle$.

Legendre transform.

$$\widehat{n}\left(\vec{r}\right) \equiv \psi^{\dagger}\left(\vec{r}\right)\psi\left(\vec{r}\right)$$

$$E\left(J\right) = \left\langle \phi_J \left| H + \int d^3r \; J\left(\vec{r}\right)\widehat{n}\left(\vec{r}\right) \right| \phi_J \right\rangle$$

$$n\left(\vec{r}\right) = \left\langle \phi_J \left| \widehat{n}\left(\vec{r}\right) \right| \phi_J \right\rangle = \frac{\delta E\left(J\right)}{\delta J\left(\vec{r}\right)}$$

The density functional is:

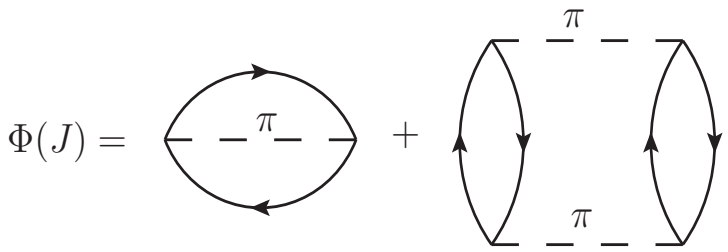
$$W\left(n\right) = E\left(J\right) - \int d^3r \; J\left(\vec{r}\right)n\left(\vec{r}\right)$$

$$\frac{\delta W\left(n\right)}{\delta n\left(\vec{r}\right)} = -J\left(\vec{r}\right)$$

When $J\left(\vec{r}\right) = 0$:

$$\frac{\delta W\left(n\right)}{\delta n\left(\vec{r}\right)} = 0 \quad n_0\left(\vec{r}\right) = \left.\frac{\delta E\left(J\right)}{\delta J\left(\vec{r}\right)}\right|_{J=0}$$

Example:

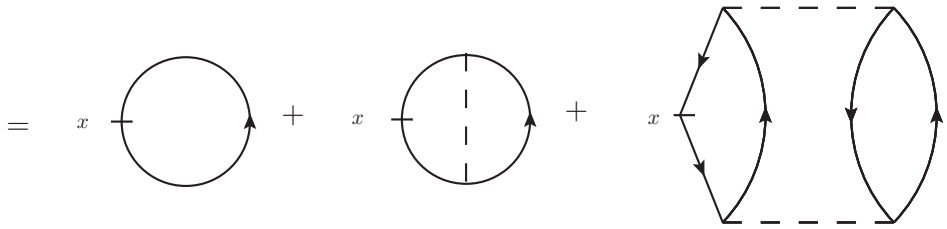


calculated with:

$$G_J^{-1} = \partial_\tau + h_0 - \mu + J \equiv G_0^{-1} + J$$

The particle density is then:

$$n(x) = -\left\langle x \left| G_J \right| x \right\rangle|_{J=0} - \left.\frac{\delta\Phi(J)}{\delta J(x)}\right|_{J=0}$$



Instead of choosing $J = 0$ as in the Legendre transform method, set:

$$J(x) = J_0(x) + J_{int}(x)$$

$$G_{J_0+J_{int}} = G_{J_0} - G_{J_0} J_{int} G_{J_0+J_{int}}$$

Density:

$$n(x) = -\langle x | G_{J_0} | x \rangle + \langle x | G_{J_0} J_{int} G_{J_0+J_{int}} | x \rangle - \frac{\delta \Phi(J)}{\delta J(x)}$$

Choose $J_0(x)$ such that the density should be given by the first term only:

$$n(x) = -\langle x | G_0 | x \rangle = \sum_{\lambda \in F} \langle \lambda | \vec{r} \rangle \langle \vec{r} | \lambda \rangle$$

$$(h_0 + J_0) | \lambda \rangle = e_\lambda | \lambda \rangle \quad Kohn - Sham\ orbits$$

$J_{int}(x)$ is determined by the equation:

$$\langle x | G_{J_0} J_{int} G_{J_0+J_{int}} | x \rangle = \frac{\delta \Phi(J)}{\delta J(x)}$$

Set $J_{int} = -J_0$ and obtain an equation for J_0:

$$\langle x | G_{J_0} J_0 G_0 | x \rangle = -\left. \frac{\delta \Phi(J)}{\delta J(x)} \right|_{J=0}$$

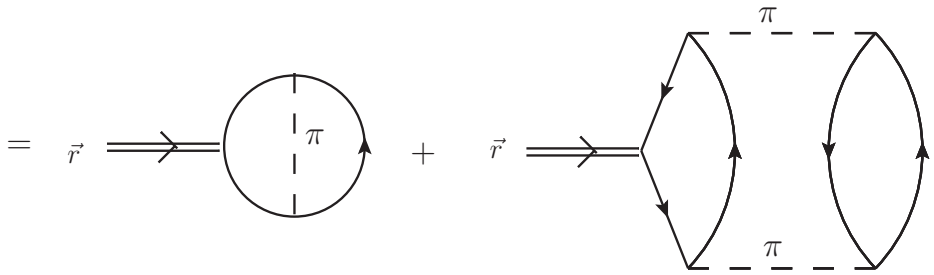
Solve $\langle x\left|G_{J_0}J_0G_0\right|x\rangle = -\left.\frac{\delta\Phi(J)}{\delta J(x)}\right|_{J=0}$ for $J_0(x)$. Write:

$$\int d^4y\,\langle x\left|G_{J_0}\right|y\rangle\,J_0(y)\,\langle y|\,G_0|\,x\rangle = -\left.\frac{\delta\Phi(J)}{\delta J(x)}\right|_{J=0}$$

$$\int d^4y\,\langle x\left|D\right|y\rangle\,J_0(y) = -\left.\frac{\delta\Phi(J)}{\delta J(x)}\right|_{J=0}$$

where $\langle x\left|D\right|y\rangle = \langle x\left|G_{J_0}\right|y\rangle\,\langle y|\,G_0|\,x\rangle$. Then:

$$J_0(x) = -\int d^4y\,\left\langle x\left|D^{-1}\right|y\right\rangle\left.\frac{\delta\Phi(J)}{\delta J(x)}\right|_{J=0}$$



Can be solved by iteration using two sets of orbits:

$$h_0\left|\lambda\right\rangle = e_\lambda\left|\lambda\right\rangle \qquad \left(h_0+J_0\right)\left|\overline{\lambda}\right\rangle = e_{\overline{\lambda}}\left|\overline{\lambda}\right\rangle$$

to calculate D and D^{-1}.

SOME REFERENCES

Diagram resummations: C.DeDominicis and P.Martin,Journ.Math.Physics 5(1964)1007

Stationary density functional and Kohn-Sham orbits: P.Hohenberg and W.Kohn, Phys.Rev.136(1964)B864

Static mean fields and stationary energy functionals: J.P.Blaizot and G.Ripka, Quantum theory of finite systems, MIT Press(1986)

Density functionals using Legendre transform: M.Valiev and G.W.Ferrando, Phys.Rev.B54(1998)9700

Density functionals for nucleons interacting with mesons: G.Ripka, arXiv:0910.1935 [nucl-th]